



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:31 AM UTC

PDB ID : 4QYJ / pdb_00004qyj
Title : Structure of Phenylacetaldehyde Dehydrogenase from Pseudomonas putida S12
Authors : Crabo, A.G.; Gassner, G.T.; Sazinsky, M.H.
Deposited on : 2014-07-24
Resolution : 2.83 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

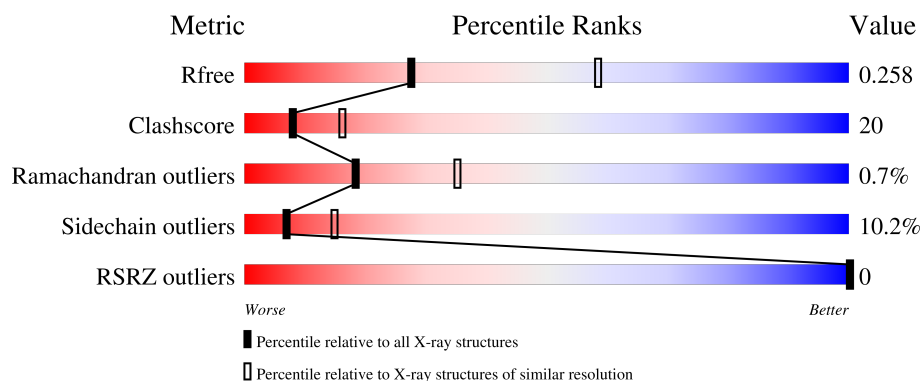
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



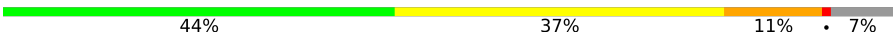
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	516	 45% 35% 13% • 7%
1	B	516	 44% 37% 11% • 7%
1	C	516	 43% 38% 12% 7%
1	D	516	 43% 36% 13% • 7%
1	E	516	 45% 36% 11% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	516	 46% 35% 11% • 7%
1	G	516	 44% 37% 11% • 7%
1	H	516	 43% 37% 12% • 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 27306 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3416	2170	580	651	15			
1	B	481	Total	C	N	O	S	0	0	0
			3411	2169	579	648	15			
1	C	481	Total	C	N	O	S	0	0	0
			3409	2167	580	647	15			
1	D	481	Total	C	N	O	S	0	0	0
			3419	2173	584	647	15			
1	E	481	Total	C	N	O	S	0	0	0
			3408	2166	580	647	15			
1	F	481	Total	C	N	O	S	0	0	0
			3411	2169	579	648	15			
1	G	481	Total	C	N	O	S	0	0	0
			3419	2172	584	648	15			
1	H	481	Total	C	N	O	S	0	0	0
			3413	2170	581	647	15			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP V4GH04
A	-18	GLY	-	expression tag	UNP V4GH04
A	-17	SER	-	expression tag	UNP V4GH04
A	-16	SER	-	expression tag	UNP V4GH04
A	-15	HIS	-	expression tag	UNP V4GH04
A	-14	HIS	-	expression tag	UNP V4GH04
A	-13	HIS	-	expression tag	UNP V4GH04
A	-12	HIS	-	expression tag	UNP V4GH04
A	-11	HIS	-	expression tag	UNP V4GH04
A	-10	HIS	-	expression tag	UNP V4GH04
A	-9	SER	-	expression tag	UNP V4GH04
A	-8	SER	-	expression tag	UNP V4GH04
A	-7	GLY	-	expression tag	UNP V4GH04

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP V4GH04
A	-5	VAL	-	expression tag	UNP V4GH04
A	-4	PRO	-	expression tag	UNP V4GH04
A	-3	ARG	-	expression tag	UNP V4GH04
A	-2	GLY	-	expression tag	UNP V4GH04
A	-1	SER	-	expression tag	UNP V4GH04
A	0	HIS	-	expression tag	UNP V4GH04
B	-19	MET	-	expression tag	UNP V4GH04
B	-18	GLY	-	expression tag	UNP V4GH04
B	-17	SER	-	expression tag	UNP V4GH04
B	-16	SER	-	expression tag	UNP V4GH04
B	-15	HIS	-	expression tag	UNP V4GH04
B	-14	HIS	-	expression tag	UNP V4GH04
B	-13	HIS	-	expression tag	UNP V4GH04
B	-12	HIS	-	expression tag	UNP V4GH04
B	-11	HIS	-	expression tag	UNP V4GH04
B	-10	HIS	-	expression tag	UNP V4GH04
B	-9	SER	-	expression tag	UNP V4GH04
B	-8	SER	-	expression tag	UNP V4GH04
B	-7	GLY	-	expression tag	UNP V4GH04
B	-6	LEU	-	expression tag	UNP V4GH04
B	-5	VAL	-	expression tag	UNP V4GH04
B	-4	PRO	-	expression tag	UNP V4GH04
B	-3	ARG	-	expression tag	UNP V4GH04
B	-2	GLY	-	expression tag	UNP V4GH04
B	-1	SER	-	expression tag	UNP V4GH04
B	0	HIS	-	expression tag	UNP V4GH04
C	-19	MET	-	expression tag	UNP V4GH04
C	-18	GLY	-	expression tag	UNP V4GH04
C	-17	SER	-	expression tag	UNP V4GH04
C	-16	SER	-	expression tag	UNP V4GH04
C	-15	HIS	-	expression tag	UNP V4GH04
C	-14	HIS	-	expression tag	UNP V4GH04
C	-13	HIS	-	expression tag	UNP V4GH04
C	-12	HIS	-	expression tag	UNP V4GH04
C	-11	HIS	-	expression tag	UNP V4GH04
C	-10	HIS	-	expression tag	UNP V4GH04
C	-9	SER	-	expression tag	UNP V4GH04
C	-8	SER	-	expression tag	UNP V4GH04
C	-7	GLY	-	expression tag	UNP V4GH04
C	-6	LEU	-	expression tag	UNP V4GH04
C	-5	VAL	-	expression tag	UNP V4GH04

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP V4GH04
C	-3	ARG	-	expression tag	UNP V4GH04
C	-2	GLY	-	expression tag	UNP V4GH04
C	-1	SER	-	expression tag	UNP V4GH04
C	0	HIS	-	expression tag	UNP V4GH04
D	-19	MET	-	expression tag	UNP V4GH04
D	-18	GLY	-	expression tag	UNP V4GH04
D	-17	SER	-	expression tag	UNP V4GH04
D	-16	SER	-	expression tag	UNP V4GH04
D	-15	HIS	-	expression tag	UNP V4GH04
D	-14	HIS	-	expression tag	UNP V4GH04
D	-13	HIS	-	expression tag	UNP V4GH04
D	-12	HIS	-	expression tag	UNP V4GH04
D	-11	HIS	-	expression tag	UNP V4GH04
D	-10	HIS	-	expression tag	UNP V4GH04
D	-9	SER	-	expression tag	UNP V4GH04
D	-8	SER	-	expression tag	UNP V4GH04
D	-7	GLY	-	expression tag	UNP V4GH04
D	-6	LEU	-	expression tag	UNP V4GH04
D	-5	VAL	-	expression tag	UNP V4GH04
D	-4	PRO	-	expression tag	UNP V4GH04
D	-3	ARG	-	expression tag	UNP V4GH04
D	-2	GLY	-	expression tag	UNP V4GH04
D	-1	SER	-	expression tag	UNP V4GH04
D	0	HIS	-	expression tag	UNP V4GH04
E	-19	MET	-	expression tag	UNP V4GH04
E	-18	GLY	-	expression tag	UNP V4GH04
E	-17	SER	-	expression tag	UNP V4GH04
E	-16	SER	-	expression tag	UNP V4GH04
E	-15	HIS	-	expression tag	UNP V4GH04
E	-14	HIS	-	expression tag	UNP V4GH04
E	-13	HIS	-	expression tag	UNP V4GH04
E	-12	HIS	-	expression tag	UNP V4GH04
E	-11	HIS	-	expression tag	UNP V4GH04
E	-10	HIS	-	expression tag	UNP V4GH04
E	-9	SER	-	expression tag	UNP V4GH04
E	-8	SER	-	expression tag	UNP V4GH04
E	-7	GLY	-	expression tag	UNP V4GH04
E	-6	LEU	-	expression tag	UNP V4GH04
E	-5	VAL	-	expression tag	UNP V4GH04
E	-4	PRO	-	expression tag	UNP V4GH04
E	-3	ARG	-	expression tag	UNP V4GH04

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP V4GH04
E	-1	SER	-	expression tag	UNP V4GH04
E	0	HIS	-	expression tag	UNP V4GH04
F	-19	MET	-	expression tag	UNP V4GH04
F	-18	GLY	-	expression tag	UNP V4GH04
F	-17	SER	-	expression tag	UNP V4GH04
F	-16	SER	-	expression tag	UNP V4GH04
F	-15	HIS	-	expression tag	UNP V4GH04
F	-14	HIS	-	expression tag	UNP V4GH04
F	-13	HIS	-	expression tag	UNP V4GH04
F	-12	HIS	-	expression tag	UNP V4GH04
F	-11	HIS	-	expression tag	UNP V4GH04
F	-10	HIS	-	expression tag	UNP V4GH04
F	-9	SER	-	expression tag	UNP V4GH04
F	-8	SER	-	expression tag	UNP V4GH04
F	-7	GLY	-	expression tag	UNP V4GH04
F	-6	LEU	-	expression tag	UNP V4GH04
F	-5	VAL	-	expression tag	UNP V4GH04
F	-4	PRO	-	expression tag	UNP V4GH04
F	-3	ARG	-	expression tag	UNP V4GH04
F	-2	GLY	-	expression tag	UNP V4GH04
F	-1	SER	-	expression tag	UNP V4GH04
F	0	HIS	-	expression tag	UNP V4GH04
G	-19	MET	-	expression tag	UNP V4GH04
G	-18	GLY	-	expression tag	UNP V4GH04
G	-17	SER	-	expression tag	UNP V4GH04
G	-16	SER	-	expression tag	UNP V4GH04
G	-15	HIS	-	expression tag	UNP V4GH04
G	-14	HIS	-	expression tag	UNP V4GH04
G	-13	HIS	-	expression tag	UNP V4GH04
G	-12	HIS	-	expression tag	UNP V4GH04
G	-11	HIS	-	expression tag	UNP V4GH04
G	-10	HIS	-	expression tag	UNP V4GH04
G	-9	SER	-	expression tag	UNP V4GH04
G	-8	SER	-	expression tag	UNP V4GH04
G	-7	GLY	-	expression tag	UNP V4GH04
G	-6	LEU	-	expression tag	UNP V4GH04
G	-5	VAL	-	expression tag	UNP V4GH04
G	-4	PRO	-	expression tag	UNP V4GH04
G	-3	ARG	-	expression tag	UNP V4GH04
G	-2	GLY	-	expression tag	UNP V4GH04
G	-1	SER	-	expression tag	UNP V4GH04

Continued on next page...

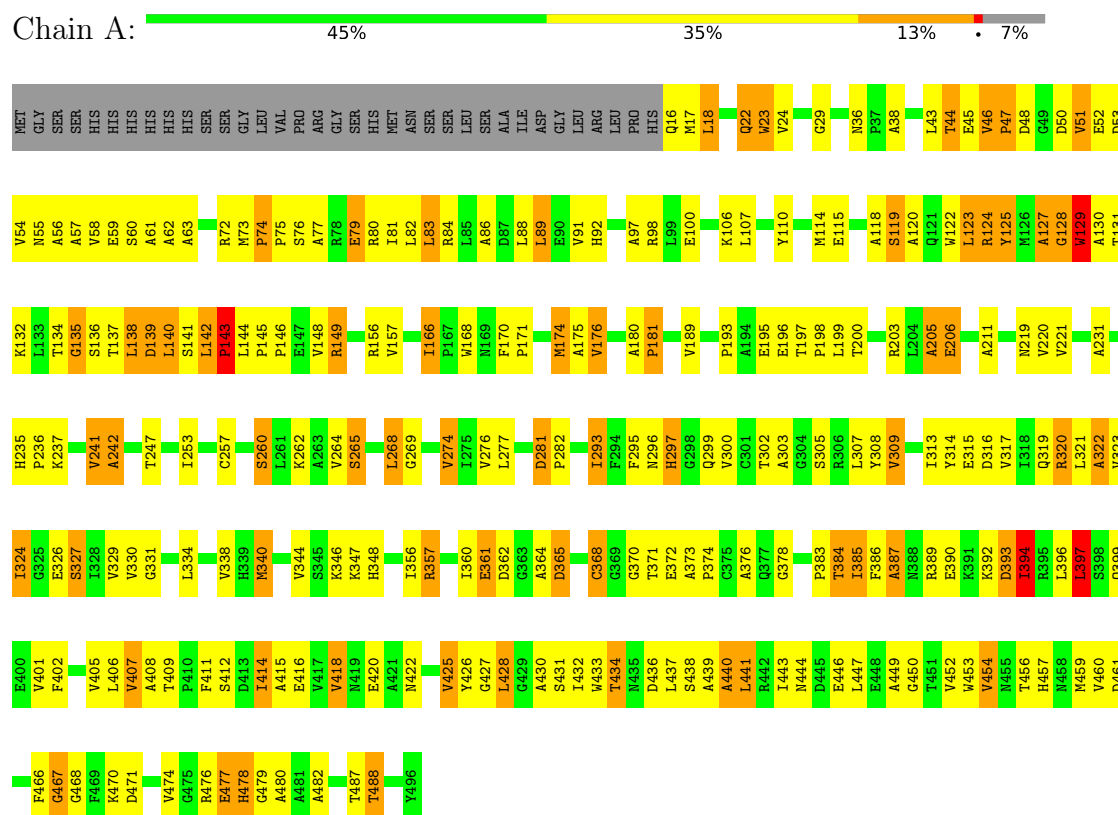
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP V4GH04
H	-19	MET	-	expression tag	UNP V4GH04
H	-18	GLY	-	expression tag	UNP V4GH04
H	-17	SER	-	expression tag	UNP V4GH04
H	-16	SER	-	expression tag	UNP V4GH04
H	-15	HIS	-	expression tag	UNP V4GH04
H	-14	HIS	-	expression tag	UNP V4GH04
H	-13	HIS	-	expression tag	UNP V4GH04
H	-12	HIS	-	expression tag	UNP V4GH04
H	-11	HIS	-	expression tag	UNP V4GH04
H	-10	HIS	-	expression tag	UNP V4GH04
H	-9	SER	-	expression tag	UNP V4GH04
H	-8	SER	-	expression tag	UNP V4GH04
H	-7	GLY	-	expression tag	UNP V4GH04
H	-6	LEU	-	expression tag	UNP V4GH04
H	-5	VAL	-	expression tag	UNP V4GH04
H	-4	PRO	-	expression tag	UNP V4GH04
H	-3	ARG	-	expression tag	UNP V4GH04
H	-2	GLY	-	expression tag	UNP V4GH04
H	-1	SER	-	expression tag	UNP V4GH04
H	0	HIS	-	expression tag	UNP V4GH04

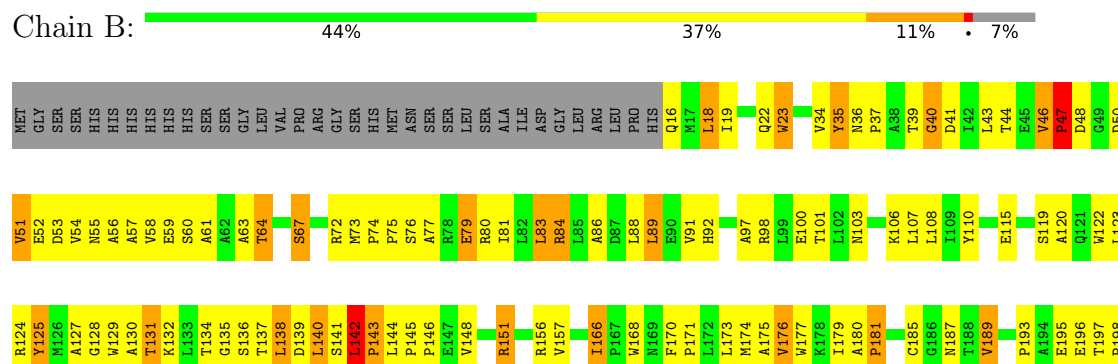
3 Residue-property plots [i](#)

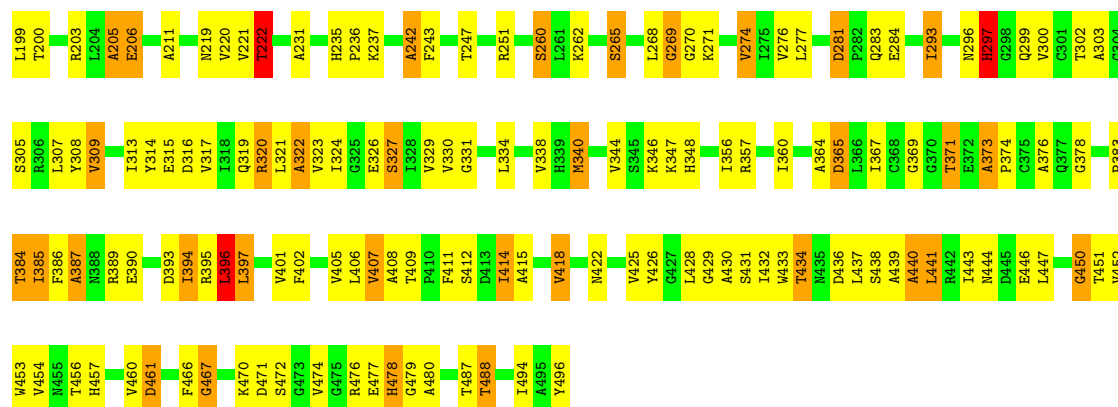
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Aldehyde dehydrogenase



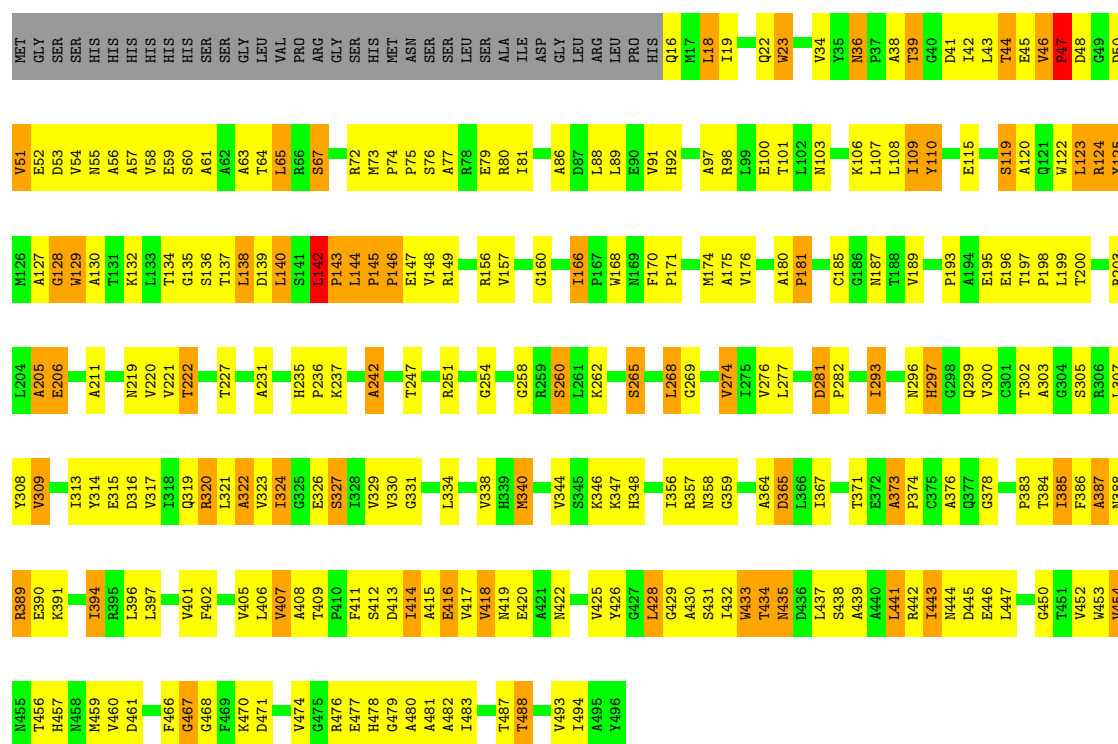
• Molecule 1: Aldehyde dehydrogenase





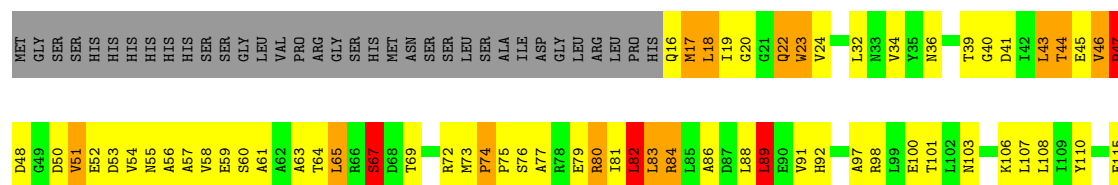
• Molecule 1: Aldehyde dehydrogenase

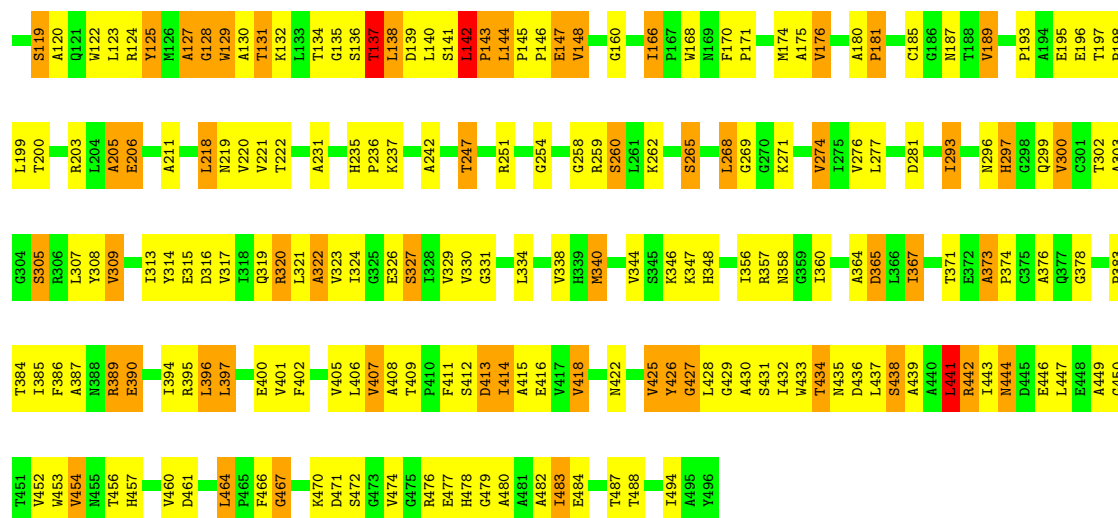
Chain C: 43% 38% 12% 7%



• Molecule 1: Aldehyde dehydrogenase

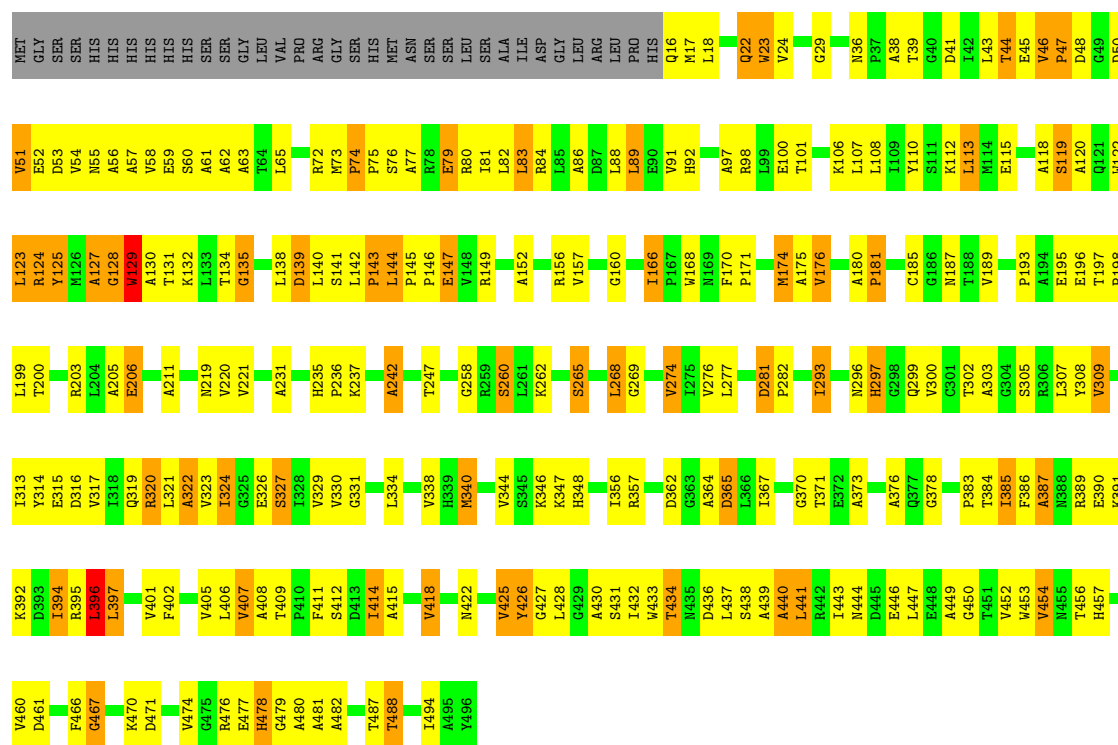
Chain D: 43% 36% 13% 7%





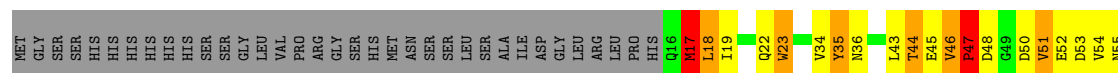
• Molecule 1: Aldehyde dehydrogenase

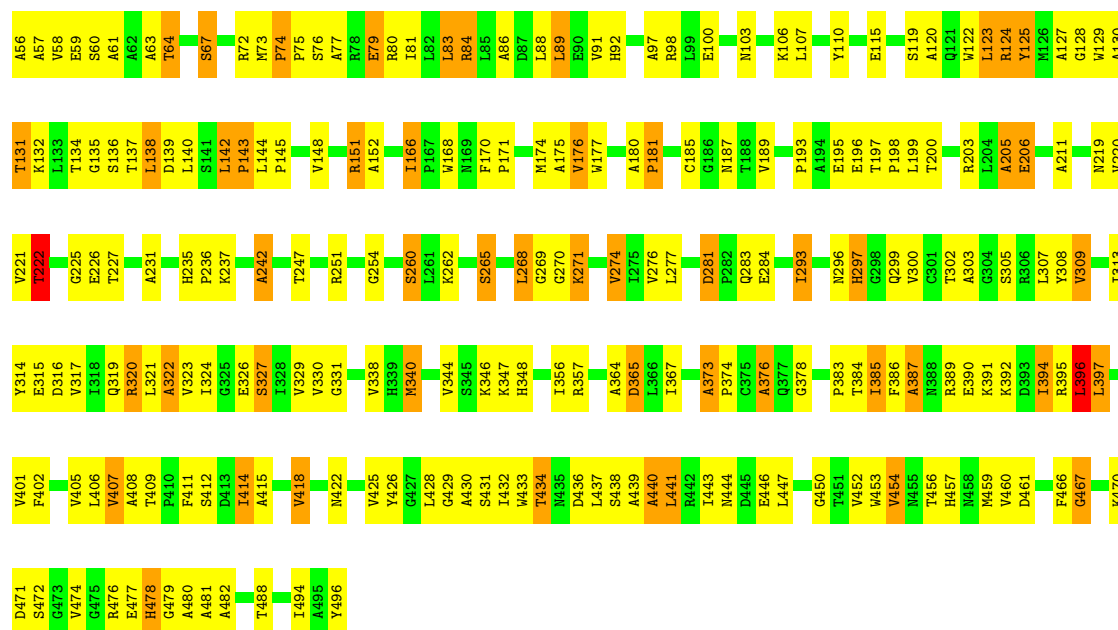
Chain E: 45% 36% 11% 7%



• Molecule 1: Aldehyde dehydrogenase

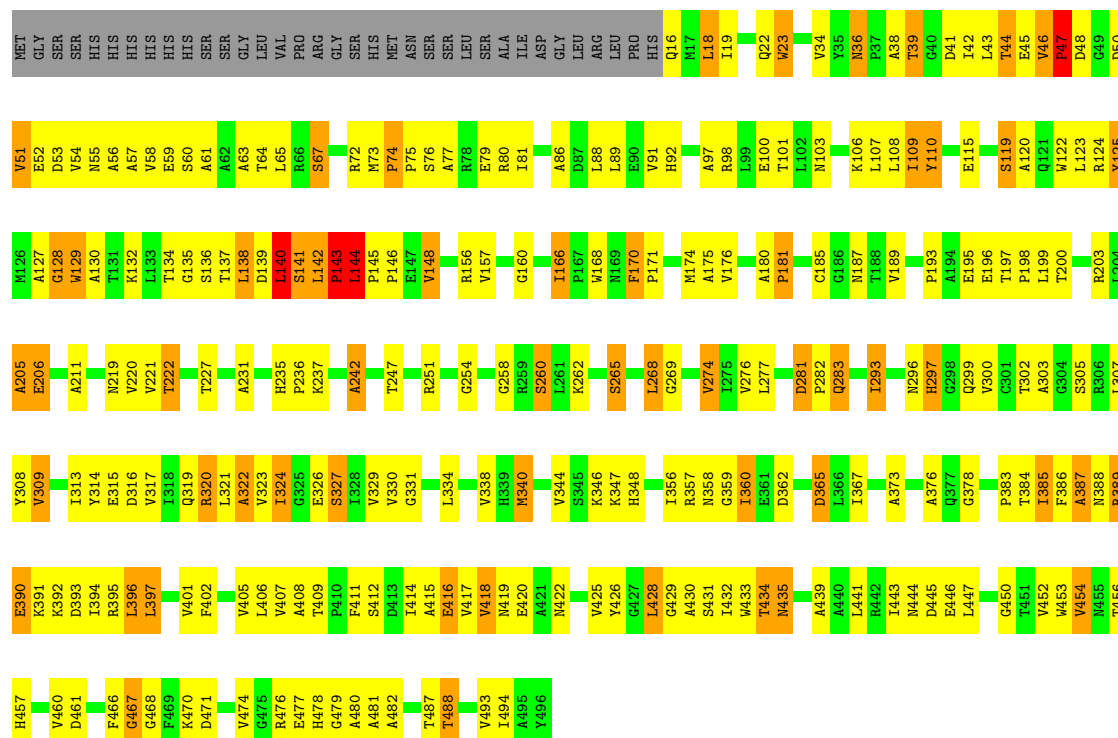
Chain F: 46% 35% 11% 7%





• Molecule 1: Aldehyde dehydrogenase

Chain G: 44% 37% 11% • 7%



• Molecule 1: Aldehyde dehydrogenase

Chain H: 43% 37% 12% • 7%

D445	Q377	G298	P198	A120	D50
D446	G378	Q299	T200	Q121	V51
		Q300		SER	GLY
G450	P383	C301	R203	L123	D53
T451	I385	A303	L204	R124	V54
V452	F386	G304	A205	Y125	N55
W453	A387	S305	E206	M126	A56
X454	R388	R306	G207	A127	HIS
Y455	R389	L307	A211	G128	HIS
Z456	E390	Y308		W129	HIS
A457	K391	V309	L218	A130	S60
	K392		N219	T131	A61
D460	V393	I313	V220	K132	A62
V461	I394	Y314	V221	L133	A63
	R395	E315	T222	T134	VAL
L464	L396	D316		G135	PRO
P465	L397	V317	G225	S136	L65
P466	E400	I318	E226	T137	ARG
G467	V401	Q319	T227	L138	GLY
K470	F402	R320	A228	D139	SER
D471		L321		L140	HIS
	V405	A322	A231	S141	MET
V474	L406	V323		L142	ASN
G475	V407	I324	H235	P143	SER
R476	A408	G325	P236	L144	SER
E477	T409	E326	K237	P145	LEU
H478	P410	S327		P146	SER
G479	F411	I328	A242	E147	ALA
A480	S412	V329		V148	ILE
A481	D413	V330	T247	A152	ASP
I482	I414	G331		L151	GLY
E484	A415	L334	R251	G160	LEU
	E416				LEU
T487	V417	V338	G254	T166	PRO
V488	V418	H339		P167	HIS
	N422	M340	G258	W168	Q16
I494	V425	V344	R259	N169	M17
Y496	Y426	S345	S260	F170	L18
	G427	K347	L261	P171	L89
L428	G429	H348	K262		I19
A430	A430	I356	S265	M174	Q22
S431	I432	R357		A175	W23
	W433	I360	L268	V176	V24
	T434	D365	L269	A180	
N435	D436	L366	G270	P181	L32
L437	L437	I367	K271	T101	N33
S438				C185	Y35
	A439		V274	L102	N36
A440	E372	D365	I275	N103	
L441	D436	L366	V276	K106	T39
R442	L437	I367	L277	L107	G40
	S438	T371	D281	L108	
	A440	E372		K192	L43
	R442	P374	I293	A194	T44
				E195	E45
				L196	V46
				C375	P47
				N296	D48
				H997	C49
				T197	S410

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.09Å 118.69Å 304.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.99 – 2.83 49.99 – 2.83	Depositor EDS
% Data completeness (in resolution range)	95.7 (49.99-2.83) 81.4 (49.99-2.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.254 , 0.258 0.254 , 0.258	Depositor DCC
R_{free} test set	4677 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 12.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27306	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.17	131/3485 (3.8%)	1.59	86/4781 (1.8%)
1	B	2.16	124/3480 (3.6%)	1.59	87/4774 (1.8%)
1	C	2.17	136/3478 (3.9%)	1.57	74/4772 (1.6%)
1	D	2.14	125/3488 (3.6%)	1.60	80/4783 (1.7%)
1	E	2.14	125/3477 (3.6%)	1.59	82/4771 (1.7%)
1	F	2.17	131/3480 (3.8%)	1.57	78/4774 (1.6%)
1	G	2.20	137/3488 (3.9%)	1.59	80/4784 (1.7%)
1	H	2.16	125/3482 (3.6%)	1.60	77/4776 (1.6%)
All	All	2.16	1034/27858 (3.7%)	1.59	644/38215 (1.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

All (1034) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	371	THR	CA-CB	-9.09	1.40	1.53
1	H	135	GLY	C-O	-8.60	1.16	1.24
1	B	135	GLY	C-O	-8.59	1.16	1.24
1	F	135	GLY	C-O	-8.58	1.16	1.24
1	E	135	GLY	C-O	-8.57	1.16	1.24
1	C	135	GLY	C-O	-8.57	1.16	1.24
1	G	135	GLY	C-O	-8.53	1.16	1.24
1	A	135	GLY	C-O	-8.52	1.16	1.24
1	D	135	GLY	C-O	-8.51	1.16	1.24
1	E	461	ASP	C-O	-8.27	1.15	1.24
1	B	281	ASP	CA-C	-8.25	1.44	1.53
1	F	281	ASP	CA-C	-8.23	1.44	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	461	ASP	C-O	-8.21	1.15	1.24
1	C	38	ALA	CA-CB	-7.80	1.41	1.53
1	G	38	ALA	CA-CB	-7.80	1.41	1.53
1	G	74	PRO	C-O	-7.49	1.18	1.25
1	C	74	PRO	C-O	-7.44	1.18	1.25
1	D	74	PRO	C-O	-7.42	1.18	1.25
1	A	74	PRO	C-O	-7.41	1.18	1.25
1	H	74	PRO	C-O	-7.41	1.18	1.25
1	B	74	PRO	C-O	-7.36	1.18	1.25
1	F	74	PRO	C-O	-7.36	1.18	1.25
1	H	365	ASP	C-O	-7.32	1.15	1.24
1	E	74	PRO	C-O	-7.32	1.18	1.25
1	D	365	ASP	C-O	-7.29	1.15	1.24
1	G	50	ASP	C-O	-7.29	1.16	1.24
1	C	50	ASP	C-O	-7.29	1.16	1.24
1	F	365	ASP	C-O	-7.29	1.15	1.24
1	F	50	ASP	C-O	-7.26	1.16	1.24
1	B	365	ASP	C-O	-7.26	1.15	1.24
1	G	365	ASP	C-O	-7.25	1.15	1.24
1	C	365	ASP	C-O	-7.25	1.15	1.24
1	E	50	ASP	C-O	-7.24	1.16	1.24
1	B	50	ASP	C-O	-7.24	1.16	1.24
1	C	119	SER	C-O	-7.24	1.15	1.24
1	E	365	ASP	C-O	-7.24	1.15	1.24
1	A	365	ASP	C-O	-7.23	1.15	1.24
1	A	50	ASP	C-O	-7.23	1.16	1.24
1	G	119	SER	C-O	-7.23	1.15	1.24
1	D	50	ASP	C-O	-7.20	1.16	1.24
1	A	119	SER	C-O	-7.18	1.15	1.24
1	E	119	SER	C-O	-7.16	1.15	1.24
1	D	119	SER	C-O	-7.16	1.15	1.24
1	H	119	SER	C-O	-7.15	1.15	1.24
1	F	181	PRO	C-O	-7.15	1.15	1.24
1	B	181	PRO	C-O	-7.14	1.15	1.24
1	H	50	ASP	C-O	-7.13	1.16	1.24
1	C	181	PRO	C-O	-7.12	1.15	1.24
1	G	181	PRO	C-O	-7.12	1.15	1.24
1	H	181	PRO	C-O	-7.09	1.15	1.24
1	E	181	PRO	C-O	-7.09	1.15	1.24
1	A	181	PRO	C-O	-7.08	1.15	1.24
1	D	181	PRO	C-O	-7.08	1.15	1.24
1	H	480	ALA	CA-CB	-7.06	1.41	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	466	PHE	C-O	-7.04	1.15	1.23
1	E	52	GLU	C-O	-7.04	1.16	1.24
1	D	480	ALA	CA-CB	-7.04	1.41	1.53
1	E	38	ALA	CA-CB	-7.04	1.42	1.53
1	B	466	PHE	C-O	-7.04	1.15	1.23
1	F	480	ALA	CA-CB	-7.03	1.41	1.53
1	G	480	ALA	CA-CB	-7.03	1.41	1.53
1	D	466	PHE	C-O	-7.02	1.15	1.23
1	C	480	ALA	CA-CB	-7.02	1.41	1.53
1	E	18	LEU	C-O	-7.01	1.16	1.24
1	A	38	ALA	CA-CB	-7.00	1.42	1.53
1	A	480	ALA	CA-CB	-7.00	1.41	1.53
1	B	480	ALA	CA-CB	-7.00	1.41	1.53
1	H	466	PHE	C-O	-7.00	1.15	1.23
1	G	432	ILE	C-O	-6.99	1.17	1.24
1	E	480	ALA	CA-CB	-6.99	1.41	1.53
1	A	52	GLU	C-O	-6.98	1.16	1.24
1	B	52	GLU	C-O	-6.98	1.16	1.24
1	F	52	GLU	C-O	-6.98	1.16	1.24
1	A	466	PHE	C-O	-6.98	1.15	1.23
1	H	52	GLU	C-O	-6.97	1.16	1.24
1	E	432	ILE	C-O	-6.96	1.17	1.24
1	D	52	GLU	C-O	-6.96	1.16	1.24
1	C	52	GLU	C-O	-6.95	1.16	1.24
1	C	466	PHE	C-O	-6.95	1.15	1.23
1	E	466	PHE	C-O	-6.94	1.15	1.23
1	G	52	GLU	C-O	-6.94	1.16	1.24
1	A	18	LEU	C-O	-6.94	1.16	1.24
1	F	432	ILE	C-O	-6.93	1.17	1.24
1	C	432	ILE	C-O	-6.91	1.17	1.24
1	G	466	PHE	C-O	-6.89	1.15	1.23
1	F	136	SER	C-O	-6.89	1.15	1.23
1	A	432	ILE	C-O	-6.89	1.17	1.24
1	D	432	ILE	C-O	-6.88	1.17	1.24
1	B	136	SER	C-O	-6.88	1.15	1.23
1	B	432	ILE	C-O	-6.87	1.17	1.24
1	H	136	SER	C-O	-6.87	1.15	1.23
1	D	136	SER	C-O	-6.86	1.15	1.23
1	A	136	SER	C-O	-6.86	1.15	1.23
1	H	432	ILE	C-O	-6.86	1.17	1.24
1	F	137	THR	C-O	-6.86	1.16	1.24
1	E	460	VAL	C-O	-6.84	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	137	THR	C-O	-6.84	1.16	1.24
1	B	137	THR	C-O	-6.84	1.16	1.24
1	E	373	ALA	CA-CB	-6.84	1.42	1.53
1	B	129	TRP	C-O	-6.83	1.15	1.24
1	G	136	SER	C-O	-6.81	1.15	1.23
1	F	129	TRP	C-O	-6.81	1.15	1.24
1	C	136	SER	C-O	-6.80	1.15	1.23
1	A	137	THR	C-O	-6.80	1.16	1.24
1	C	137	THR	C-O	-6.80	1.16	1.24
1	C	303	ALA	C-O	-6.79	1.15	1.23
1	D	137	THR	C-O	-6.79	1.16	1.24
1	C	450	GLY	C-O	-6.79	1.16	1.24
1	G	450	GLY	C-O	-6.78	1.16	1.24
1	H	137	THR	C-O	-6.78	1.16	1.24
1	F	303	ALA	C-O	-6.77	1.15	1.23
1	A	460	VAL	C-O	-6.77	1.17	1.24
1	B	303	ALA	C-O	-6.77	1.15	1.23
1	D	387	ALA	C-O	-6.76	1.15	1.24
1	G	303	ALA	C-O	-6.76	1.15	1.23
1	H	387	ALA	C-O	-6.76	1.15	1.24
1	E	387	ALA	C-O	-6.75	1.15	1.24
1	F	387	ALA	C-O	-6.75	1.15	1.24
1	A	303	ALA	C-O	-6.75	1.15	1.23
1	A	387	ALA	C-O	-6.75	1.15	1.24
1	D	406	LEU	C-O	-6.75	1.15	1.24
1	E	450	GLY	C-O	-6.73	1.16	1.24
1	G	406	LEU	C-O	-6.73	1.15	1.24
1	A	450	GLY	C-O	-6.72	1.16	1.24
1	B	387	ALA	C-O	-6.72	1.15	1.24
1	E	303	ALA	C-O	-6.72	1.15	1.23
1	H	406	LEU	C-O	-6.72	1.15	1.24
1	C	406	LEU	C-O	-6.72	1.15	1.24
1	D	303	ALA	C-O	-6.71	1.15	1.23
1	F	450	GLY	C-O	-6.71	1.16	1.24
1	A	406	LEU	C-O	-6.71	1.15	1.24
1	B	450	GLY	C-O	-6.71	1.16	1.24
1	F	220	VAL	C-O	-6.71	1.16	1.24
1	D	450	GLY	C-O	-6.71	1.16	1.24
1	H	97	ALA	C-O	-6.68	1.16	1.24
1	H	303	ALA	C-O	-6.68	1.15	1.23
1	G	97	ALA	C-O	-6.67	1.16	1.24
1	F	406	LEU	C-O	-6.66	1.15	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	270	GLY	C-O	-6.66	1.17	1.23
1	E	406	LEU	C-O	-6.66	1.15	1.24
1	B	220	VAL	C-O	-6.66	1.17	1.24
1	H	220	VAL	C-O	-6.65	1.17	1.24
1	H	450	GLY	C-O	-6.65	1.16	1.24
1	B	406	LEU	C-O	-6.65	1.15	1.24
1	D	220	VAL	C-O	-6.64	1.17	1.24
1	G	220	VAL	C-O	-6.64	1.17	1.24
1	C	97	ALA	C-O	-6.64	1.16	1.24
1	F	120	ALA	C-O	-6.64	1.15	1.24
1	C	220	VAL	C-O	-6.63	1.17	1.24
1	A	393	ASP	CA-C	-6.62	1.46	1.53
1	B	120	ALA	C-O	-6.62	1.15	1.24
1	B	407	VAL	C-O	-6.62	1.16	1.24
1	H	242	ALA	CA-CB	-6.62	1.44	1.53
1	A	220	VAL	C-O	-6.61	1.17	1.24
1	F	407	VAL	C-O	-6.61	1.16	1.24
1	D	120	ALA	C-O	-6.61	1.15	1.24
1	D	97	ALA	C-O	-6.60	1.16	1.24
1	G	242	ALA	CA-CB	-6.60	1.44	1.53
1	G	407	VAL	C-O	-6.60	1.16	1.24
1	E	309	VAL	C-O	-6.60	1.17	1.24
1	F	309	VAL	C-O	-6.60	1.17	1.24
1	C	242	ALA	CA-CB	-6.59	1.44	1.53
1	B	97	ALA	C-O	-6.59	1.16	1.24
1	H	407	VAL	C-O	-6.59	1.16	1.24
1	A	97	ALA	C-O	-6.58	1.16	1.24
1	D	309	VAL	C-O	-6.58	1.17	1.24
1	C	407	VAL	C-O	-6.58	1.16	1.24
1	D	407	VAL	C-O	-6.58	1.16	1.24
1	G	309	VAL	C-O	-6.58	1.17	1.24
1	A	309	VAL	C-O	-6.58	1.17	1.24
1	F	242	ALA	CA-CB	-6.58	1.44	1.53
1	E	407	VAL	C-O	-6.58	1.16	1.24
1	C	309	VAL	C-O	-6.57	1.17	1.24
1	E	220	VAL	C-O	-6.57	1.17	1.24
1	A	407	VAL	C-O	-6.56	1.16	1.24
1	H	120	ALA	C-O	-6.56	1.15	1.24
1	E	242	ALA	CA-CB	-6.56	1.44	1.53
1	B	242	ALA	CA-CB	-6.56	1.44	1.53
1	A	242	ALA	CA-CB	-6.55	1.44	1.53
1	F	97	ALA	C-O	-6.55	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	242	ALA	CA-CB	-6.55	1.44	1.53
1	E	97	ALA	C-O	-6.55	1.16	1.24
1	H	309	VAL	C-O	-6.54	1.17	1.24
1	B	309	VAL	C-O	-6.54	1.17	1.24
1	A	120	ALA	C-O	-6.54	1.15	1.24
1	G	434	THR	N-CA	-6.53	1.38	1.46
1	A	149	ARG	C-O	-6.53	1.15	1.23
1	C	434	THR	N-CA	-6.52	1.38	1.46
1	A	426	TYR	C-O	-6.51	1.15	1.23
1	E	120	ALA	C-O	-6.50	1.15	1.24
1	C	120	ALA	C-O	-6.48	1.16	1.24
1	B	460	VAL	C-O	-6.48	1.17	1.24
1	F	443	ILE	C-O	-6.48	1.16	1.24
1	H	460	VAL	C-O	-6.47	1.17	1.24
1	D	460	VAL	C-O	-6.46	1.17	1.24
1	F	460	VAL	C-O	-6.46	1.17	1.24
1	G	120	ALA	C-O	-6.45	1.16	1.24
1	C	460	VAL	C-O	-6.44	1.17	1.24
1	A	443	ILE	C-O	-6.44	1.16	1.24
1	F	281	ASP	C-O	-6.41	1.15	1.23
1	E	242	ALA	C-O	-6.39	1.16	1.23
1	B	443	ILE	C-O	-6.39	1.17	1.24
1	E	443	ILE	C-O	-6.39	1.17	1.24
1	G	443	ILE	C-O	-6.38	1.17	1.24
1	C	443	ILE	C-O	-6.37	1.17	1.24
1	F	242	ALA	C-O	-6.37	1.16	1.23
1	A	63	ALA	CA-CB	-6.37	1.43	1.53
1	B	242	ALA	C-O	-6.36	1.16	1.23
1	F	454	VAL	C-O	-6.36	1.17	1.24
1	F	408	ALA	C-O	-6.36	1.16	1.24
1	A	242	ALA	C-O	-6.36	1.16	1.23
1	G	460	VAL	C-O	-6.36	1.17	1.24
1	G	124	ARG	C-O	-6.35	1.16	1.24
1	G	144	LEU	CA-C	-6.35	1.44	1.52
1	E	63	ALA	CA-CB	-6.35	1.43	1.53
1	C	124	ARG	C-O	-6.34	1.16	1.24
1	B	281	ASP	C-O	-6.34	1.15	1.23
1	D	203	ARG	C-O	-6.34	1.16	1.24
1	H	203	ARG	C-O	-6.33	1.16	1.24
1	A	454	VAL	C-O	-6.33	1.17	1.24
1	D	124	ARG	C-O	-6.33	1.16	1.24
1	G	454	VAL	C-O	-6.33	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	124	ARG	C-O	-6.33	1.16	1.24
1	F	124	ARG	C-O	-6.33	1.16	1.24
1	D	242	ALA	C-O	-6.32	1.16	1.23
1	C	454	VAL	C-O	-6.32	1.17	1.24
1	E	124	ARG	C-O	-6.32	1.16	1.24
1	H	124	ARG	C-O	-6.32	1.16	1.24
1	H	242	ALA	C-O	-6.32	1.16	1.23
1	B	408	ALA	C-O	-6.31	1.16	1.24
1	E	408	ALA	C-O	-6.30	1.16	1.24
1	A	124	ARG	C-O	-6.30	1.16	1.24
1	C	203	ARG	C-O	-6.30	1.16	1.24
1	D	408	ALA	C-O	-6.30	1.16	1.24
1	D	454	VAL	C-O	-6.29	1.17	1.24
1	C	242	ALA	C-O	-6.29	1.16	1.23
1	G	447	LEU	C-O	-6.29	1.15	1.23
1	F	447	LEU	C-O	-6.29	1.15	1.23
1	E	454	VAL	C-O	-6.29	1.17	1.24
1	B	454	VAL	C-O	-6.29	1.17	1.24
1	B	203	ARG	C-O	-6.28	1.16	1.24
1	G	242	ALA	C-O	-6.28	1.16	1.23
1	G	408	ALA	C-O	-6.28	1.16	1.24
1	H	408	ALA	CA-CB	-6.28	1.43	1.53
1	A	203	ARG	C-O	-6.28	1.16	1.24
1	D	408	ALA	CA-CB	-6.27	1.43	1.53
1	D	447	LEU	C-O	-6.27	1.15	1.23
1	E	92	HIS	CA-C	-6.27	1.45	1.53
1	E	447	LEU	C-O	-6.27	1.15	1.23
1	H	408	ALA	C-O	-6.27	1.16	1.24
1	E	408	ALA	CA-CB	-6.26	1.43	1.53
1	A	92	HIS	CA-C	-6.26	1.45	1.53
1	F	63	ALA	CA-CB	-6.25	1.43	1.53
1	B	63	ALA	CA-CB	-6.25	1.43	1.53
1	E	203	ARG	C-O	-6.25	1.16	1.24
1	H	454	VAL	C-O	-6.25	1.17	1.24
1	C	408	ALA	C-O	-6.25	1.17	1.24
1	F	92	HIS	CA-C	-6.25	1.45	1.53
1	A	408	ALA	C-O	-6.25	1.17	1.24
1	A	447	LEU	C-O	-6.25	1.16	1.23
1	C	447	LEU	C-O	-6.25	1.16	1.23
1	G	203	ARG	C-O	-6.25	1.16	1.24
1	F	203	ARG	C-O	-6.24	1.16	1.24
1	H	393	ASP	CA-C	-6.24	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	92	HIS	CA-C	-6.24	1.45	1.53
1	D	92	HIS	CA-C	-6.24	1.45	1.53
1	H	447	LEU	C-O	-6.24	1.16	1.23
1	A	408	ALA	CA-CB	-6.23	1.43	1.53
1	B	92	HIS	CA-C	-6.22	1.45	1.53
1	C	435	ASN	CA-C	-6.22	1.44	1.53
1	G	92	HIS	CA-C	-6.22	1.45	1.53
1	E	22	GLN	C-O	-6.22	1.16	1.24
1	B	447	LEU	C-O	-6.22	1.16	1.23
1	G	435	ASN	CA-C	-6.21	1.44	1.53
1	B	408	ALA	CA-CB	-6.21	1.44	1.53
1	C	92	HIS	CA-C	-6.21	1.45	1.53
1	B	22	GLN	C-O	-6.20	1.16	1.24
1	A	22	GLN	C-O	-6.19	1.16	1.24
1	F	22	GLN	C-O	-6.18	1.16	1.24
1	C	408	ALA	CA-CB	-6.18	1.44	1.53
1	G	283	GLN	C-O	-6.17	1.16	1.24
1	F	408	ALA	CA-CB	-6.16	1.44	1.53
1	G	408	ALA	CA-CB	-6.14	1.44	1.53
1	H	347	LYS	C-O	-6.14	1.16	1.24
1	D	22	GLN	C-O	-6.13	1.16	1.24
1	B	418	VAL	C-O	-6.11	1.16	1.24
1	H	434	THR	C-O	-6.11	1.17	1.23
1	D	434	THR	C-O	-6.11	1.17	1.23
1	E	347	LYS	C-O	-6.11	1.16	1.24
1	E	315	GLU	C-O	-6.11	1.17	1.24
1	F	409	THR	C-O	-6.10	1.16	1.24
1	A	347	LYS	C-O	-6.10	1.16	1.24
1	H	315	GLU	C-O	-6.10	1.17	1.24
1	E	430	ALA	C-O	-6.10	1.16	1.23
1	F	418	VAL	C-O	-6.10	1.16	1.24
1	A	430	ALA	C-O	-6.10	1.16	1.23
1	D	315	GLU	C-O	-6.10	1.17	1.24
1	F	457	HIS	C-O	-6.10	1.16	1.23
1	H	430	ALA	C-O	-6.10	1.16	1.23
1	G	439	ALA	CA-CB	-6.09	1.43	1.53
1	G	347	LYS	C-O	-6.09	1.16	1.24
1	B	347	LYS	C-O	-6.09	1.16	1.24
1	D	430	ALA	C-O	-6.09	1.16	1.23
1	H	22	GLN	C-O	-6.09	1.16	1.24
1	D	347	LYS	C-O	-6.09	1.16	1.24
1	F	430	ALA	C-O	-6.08	1.16	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	418	VAL	C-O	-6.08	1.17	1.24
1	F	347	LYS	C-O	-6.08	1.16	1.24
1	C	439	ALA	CA-CB	-6.08	1.44	1.53
1	A	315	GLU	C-O	-6.07	1.17	1.24
1	E	439	ALA	CA-CB	-6.07	1.43	1.53
1	H	418	VAL	C-O	-6.07	1.17	1.24
1	B	315	GLU	C-O	-6.07	1.17	1.24
1	F	439	ALA	CA-CB	-6.07	1.43	1.53
1	C	347	LYS	C-O	-6.07	1.16	1.24
1	D	457	HIS	C-O	-6.07	1.16	1.23
1	G	457	HIS	C-O	-6.07	1.16	1.23
1	F	221	VAL	C-O	-6.06	1.16	1.24
1	H	439	ALA	CA-CB	-6.06	1.44	1.53
1	A	457	HIS	C-O	-6.06	1.16	1.23
1	B	409	THR	C-O	-6.05	1.16	1.24
1	C	430	ALA	C-O	-6.05	1.16	1.23
1	A	418	VAL	C-O	-6.05	1.17	1.24
1	B	430	ALA	C-O	-6.04	1.16	1.23
1	C	315	GLU	C-O	-6.04	1.17	1.24
1	H	221	VAL	C-O	-6.04	1.16	1.24
1	B	439	ALA	CA-CB	-6.04	1.44	1.53
1	B	457	HIS	C-O	-6.04	1.16	1.23
1	B	221	VAL	C-O	-6.04	1.16	1.24
1	G	387	ALA	C-O	-6.04	1.16	1.24
1	H	457	HIS	C-O	-6.04	1.16	1.23
1	A	439	ALA	CA-CB	-6.04	1.44	1.53
1	E	409	THR	C-O	-6.04	1.16	1.24
1	A	221	VAL	C-O	-6.03	1.16	1.24
1	F	315	GLU	C-O	-6.03	1.17	1.24
1	D	439	ALA	CA-CB	-6.03	1.44	1.53
1	A	409	THR	C-O	-6.03	1.16	1.24
1	A	433	TRP	C-O	-6.03	1.17	1.24
1	D	433	TRP	C-O	-6.03	1.17	1.24
1	G	430	ALA	C-O	-6.03	1.16	1.23
1	E	433	TRP	C-O	-6.03	1.17	1.24
1	G	221	VAL	C-O	-6.03	1.16	1.24
1	D	221	VAL	C-O	-6.02	1.16	1.24
1	E	86	ALA	CA-CB	-6.02	1.43	1.53
1	C	387	ALA	C-O	-6.02	1.16	1.24
1	D	63	ALA	CA-CB	-6.02	1.43	1.53
1	C	457	HIS	C-O	-6.01	1.16	1.23
1	E	221	VAL	C-O	-6.01	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	221	VAL	C-O	-6.01	1.16	1.24
1	E	457	HIS	C-O	-6.01	1.16	1.23
1	G	63	ALA	CA-CB	-6.01	1.43	1.53
1	D	409	THR	C-O	-6.00	1.16	1.24
1	C	433	TRP	C-O	-6.00	1.17	1.24
1	C	409	THR	C-O	-6.00	1.16	1.24
1	H	63	ALA	CA-CB	-6.00	1.43	1.53
1	C	63	ALA	CA-CB	-6.00	1.43	1.53
1	C	219	ASN	C-O	-6.00	1.16	1.23
1	G	315	GLU	C-O	-6.00	1.17	1.24
1	H	409	THR	C-O	-6.00	1.16	1.24
1	G	418	VAL	C-O	-6.00	1.17	1.24
1	G	409	THR	C-O	-5.99	1.16	1.24
1	F	433	TRP	C-O	-5.99	1.17	1.24
1	E	470	LYS	C-O	-5.99	1.19	1.24
1	C	418	VAL	C-O	-5.99	1.17	1.24
1	G	219	ASN	C-O	-5.99	1.16	1.23
1	A	394	ILE	CA-C	-5.98	1.45	1.52
1	B	433	TRP	C-O	-5.98	1.17	1.24
1	G	433	TRP	C-O	-5.98	1.17	1.24
1	G	134	THR	C-O	-5.98	1.16	1.23
1	A	219	ASN	C-O	-5.98	1.16	1.23
1	E	488	THR	C-O	-5.98	1.16	1.24
1	A	86	ALA	CA-CB	-5.98	1.43	1.53
1	C	488	THR	C-O	-5.98	1.16	1.24
1	E	418	VAL	C-O	-5.97	1.17	1.24
1	E	46	VAL	C-O	-5.97	1.16	1.24
1	E	219	ASN	C-O	-5.97	1.16	1.23
1	D	470	LYS	C-O	-5.97	1.19	1.24
1	C	46	VAL	C-O	-5.97	1.16	1.24
1	D	219	ASN	C-O	-5.97	1.16	1.23
1	F	46	VAL	C-O	-5.97	1.16	1.24
1	G	46	VAL	C-O	-5.96	1.17	1.24
1	G	59	GLU	CA-C	-5.96	1.44	1.52
1	H	433	TRP	C-O	-5.96	1.17	1.24
1	H	470	LYS	C-O	-5.95	1.19	1.24
1	A	488	THR	C-O	-5.95	1.16	1.24
1	F	219	ASN	C-O	-5.95	1.16	1.23
1	H	46	VAL	C-O	-5.94	1.17	1.24
1	B	46	VAL	C-O	-5.94	1.17	1.24
1	A	46	VAL	C-O	-5.93	1.17	1.24
1	H	488	THR	C-O	-5.92	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	470	LYS	C-O	-5.92	1.19	1.24
1	B	219	ASN	C-O	-5.92	1.16	1.23
1	D	46	VAL	C-O	-5.92	1.17	1.24
1	F	470	LYS	C-O	-5.91	1.19	1.24
1	G	488	THR	C-O	-5.91	1.16	1.24
1	F	86	ALA	CA-CB	-5.91	1.43	1.53
1	F	488	THR	C-O	-5.91	1.16	1.24
1	H	219	ASN	C-O	-5.91	1.16	1.23
1	C	134	THR	C-O	-5.91	1.16	1.23
1	D	488	THR	C-O	-5.90	1.16	1.24
1	G	86	ALA	CA-CB	-5.90	1.43	1.53
1	C	59	GLU	CA-C	-5.90	1.44	1.52
1	B	488	THR	C-O	-5.89	1.16	1.24
1	F	452	VAL	C-O	-5.89	1.16	1.24
1	C	86	ALA	CA-CB	-5.89	1.43	1.53
1	D	86	ALA	CA-CB	-5.89	1.43	1.53
1	G	22	GLN	C-O	-5.89	1.16	1.24
1	C	39	THR	C-O	-5.89	1.17	1.23
1	C	470	LYS	C-O	-5.89	1.19	1.24
1	H	86	ALA	CA-CB	-5.88	1.43	1.53
1	A	134	THR	C-O	-5.88	1.16	1.23
1	G	39	THR	C-O	-5.88	1.17	1.23
1	G	53	ASP	C-O	-5.88	1.16	1.24
1	B	470	LYS	C-O	-5.87	1.19	1.24
1	E	134	THR	C-O	-5.87	1.16	1.23
1	B	86	ALA	CA-CB	-5.87	1.43	1.53
1	F	77	ALA	CA-CB	-5.87	1.44	1.53
1	G	77	ALA	CA-CB	-5.87	1.44	1.53
1	F	373	ALA	CA-CB	-5.87	1.42	1.52
1	G	470	LYS	C-O	-5.86	1.19	1.24
1	C	77	ALA	CA-CB	-5.86	1.44	1.53
1	C	322	ALA	CA-CB	-5.86	1.43	1.53
1	D	77	ALA	CA-CB	-5.86	1.44	1.53
1	G	373	ALA	CA-CB	-5.86	1.42	1.52
1	B	59	GLU	CA-C	-5.85	1.44	1.52
1	D	308	TYR	C-O	-5.85	1.17	1.24
1	D	322	ALA	CA-CB	-5.85	1.43	1.53
1	A	452	VAL	C-O	-5.85	1.16	1.24
1	B	452	VAL	C-O	-5.85	1.16	1.24
1	E	322	ALA	CA-CB	-5.85	1.43	1.53
1	A	322	ALA	CA-CB	-5.85	1.43	1.53
1	B	373	ALA	CA-CB	-5.84	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	373	ALA	CA-CB	-5.84	1.42	1.52
1	F	83	LEU	C-O	-5.84	1.17	1.24
1	F	478	HIS	C-O	-5.84	1.15	1.24
1	H	77	ALA	CA-CB	-5.84	1.44	1.53
1	C	22	GLN	C-O	-5.84	1.16	1.24
1	G	452	VAL	C-O	-5.84	1.16	1.24
1	E	308	TYR	C-O	-5.83	1.17	1.24
1	B	134	THR	C-O	-5.83	1.16	1.23
1	C	373	ALA	CA-CB	-5.83	1.42	1.52
1	E	452	VAL	C-O	-5.83	1.16	1.24
1	H	478	HIS	C-O	-5.83	1.15	1.24
1	A	59	GLU	CA-C	-5.83	1.45	1.52
1	B	322	ALA	CA-CB	-5.83	1.43	1.53
1	H	452	VAL	C-O	-5.83	1.16	1.24
1	B	83	LEU	C-O	-5.83	1.17	1.24
1	E	77	ALA	CA-CB	-5.83	1.44	1.53
1	A	77	ALA	CA-CB	-5.82	1.44	1.53
1	B	478	HIS	C-O	-5.82	1.15	1.24
1	G	322	ALA	CA-CB	-5.82	1.43	1.53
1	H	322	ALA	CA-CB	-5.82	1.43	1.53
1	C	53	ASP	C-O	-5.82	1.16	1.24
1	D	452	VAL	C-O	-5.82	1.16	1.24
1	H	373	ALA	CA-CB	-5.82	1.42	1.52
1	G	453	TRP	C-O	-5.82	1.16	1.23
1	B	77	ALA	CA-CB	-5.82	1.44	1.53
1	D	134	THR	C-O	-5.82	1.16	1.23
1	F	322	ALA	CA-CB	-5.81	1.43	1.53
1	E	53	ASP	C-O	-5.81	1.16	1.24
1	F	59	GLU	CA-C	-5.81	1.45	1.52
1	E	59	GLU	CA-C	-5.80	1.45	1.52
1	A	308	TYR	C-O	-5.80	1.17	1.24
1	F	134	THR	C-O	-5.80	1.16	1.23
1	F	271	LYS	C-O	-5.80	1.16	1.23
1	H	356	ILE	C-O	-5.80	1.17	1.24
1	E	143	PRO	N-CD	5.80	1.55	1.47
1	D	478	HIS	C-O	-5.79	1.15	1.24
1	E	370	GLY	C-O	-5.79	1.19	1.23
1	H	134	THR	C-O	-5.79	1.16	1.23
1	A	53	ASP	C-O	-5.79	1.16	1.24
1	B	53	ASP	C-O	-5.78	1.16	1.24
1	C	308	TYR	C-O	-5.78	1.17	1.24
1	C	452	VAL	C-O	-5.78	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	308	TYR	C-O	-5.78	1.17	1.24
1	H	59	GLU	CA-C	-5.78	1.45	1.52
1	F	386	PHE	C-O	-5.78	1.17	1.24
1	D	59	GLU	CA-C	-5.77	1.45	1.52
1	D	356	ILE	C-O	-5.77	1.17	1.24
1	B	308	TYR	C-O	-5.77	1.17	1.24
1	H	53	ASP	C-O	-5.77	1.16	1.24
1	H	376	ALA	CA-CB	-5.77	1.44	1.53
1	H	308	TYR	C-O	-5.76	1.17	1.24
1	D	53	ASP	C-O	-5.76	1.16	1.24
1	C	376	ALA	CA-CB	-5.75	1.44	1.53
1	D	453	TRP	C-O	-5.75	1.16	1.23
1	F	130	ALA	CA-CB	-5.75	1.44	1.53
1	A	453	TRP	C-O	-5.75	1.16	1.23
1	A	376	ALA	CA-CB	-5.75	1.44	1.53
1	D	376	ALA	CA-CB	-5.75	1.44	1.53
1	F	376	ALA	CA-CB	-5.75	1.44	1.53
1	F	53	ASP	C-O	-5.75	1.16	1.24
1	B	453	TRP	C-O	-5.75	1.16	1.23
1	G	376	ALA	CA-CB	-5.74	1.44	1.53
1	B	130	ALA	CA-CB	-5.74	1.44	1.53
1	C	453	TRP	C-O	-5.74	1.16	1.23
1	H	453	TRP	C-O	-5.74	1.16	1.23
1	B	386	PHE	C-O	-5.74	1.17	1.24
1	A	356	ILE	C-O	-5.74	1.17	1.24
1	B	376	ALA	CA-CB	-5.73	1.44	1.53
1	G	146	PRO	N-CD	-5.73	1.39	1.47
1	E	356	ILE	C-O	-5.72	1.17	1.24
1	E	376	ALA	CA-CB	-5.72	1.44	1.53
1	A	143	PRO	N-CD	5.72	1.55	1.47
1	B	356	ILE	C-O	-5.72	1.17	1.24
1	C	100	GLU	C-O	-5.71	1.16	1.24
1	E	100	GLU	C-O	-5.71	1.16	1.24
1	C	356	ILE	C-O	-5.71	1.17	1.24
1	F	453	TRP	C-O	-5.71	1.17	1.23
1	B	100	GLU	C-O	-5.71	1.16	1.24
1	D	386	PHE	C-O	-5.71	1.17	1.24
1	F	308	TYR	C-O	-5.70	1.17	1.24
1	D	67	SER	C-O	-5.70	1.16	1.23
1	E	453	TRP	C-O	-5.70	1.17	1.23
1	A	386	PHE	C-O	-5.69	1.17	1.24
1	H	130	ALA	CA-CB	-5.68	1.43	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	67	SER	C-O	-5.68	1.16	1.23
1	A	100	GLU	C-O	-5.68	1.16	1.24
1	C	331	GLY	C-O	-5.68	1.17	1.23
1	H	386	PHE	C-O	-5.68	1.17	1.24
1	B	331	GLY	C-O	-5.68	1.17	1.23
1	F	356	ILE	C-O	-5.68	1.17	1.24
1	G	356	ILE	C-O	-5.67	1.17	1.24
1	D	100	GLU	C-O	-5.67	1.16	1.24
1	G	305	SER	CA-C	-5.67	1.45	1.52
1	G	100	GLU	C-O	-5.67	1.16	1.24
1	H	100	GLU	C-O	-5.66	1.16	1.24
1	A	331	GLY	C-O	-5.66	1.17	1.23
1	C	386	PHE	C-O	-5.66	1.17	1.24
1	G	36	ASN	C-O	-5.66	1.18	1.24
1	H	331	GLY	C-O	-5.66	1.17	1.23
1	E	386	PHE	C-O	-5.65	1.17	1.24
1	E	482	ALA	CA-CB	-5.65	1.44	1.53
1	G	331	GLY	C-O	-5.65	1.17	1.23
1	H	18	LEU	C-O	-5.65	1.17	1.24
1	F	100	GLU	C-O	-5.65	1.16	1.24
1	C	36	ASN	C-O	-5.65	1.18	1.24
1	D	18	LEU	C-O	-5.65	1.17	1.24
1	F	331	GLY	C-O	-5.65	1.17	1.23
1	D	144	LEU	CA-C	-5.65	1.45	1.52
1	E	305	SER	CA-C	-5.64	1.45	1.52
1	D	130	ALA	CA-CB	-5.64	1.43	1.53
1	G	67	SER	C-O	-5.64	1.16	1.23
1	B	305	SER	CA-C	-5.64	1.45	1.52
1	D	79	GLU	C-O	-5.64	1.16	1.24
1	D	331	GLY	C-O	-5.64	1.17	1.23
1	H	79	GLU	C-O	-5.64	1.16	1.24
1	A	305	SER	CA-C	-5.64	1.45	1.52
1	C	305	SER	CA-C	-5.64	1.45	1.52
1	C	18	LEU	C-O	-5.63	1.17	1.24
1	G	387	ALA	CA-CB	-5.63	1.45	1.53
1	G	386	PHE	C-O	-5.62	1.17	1.24
1	E	331	GLY	C-O	-5.62	1.17	1.23
1	H	305	SER	CA-C	-5.62	1.45	1.52
1	G	478	HIS	C-O	-5.62	1.15	1.23
1	H	461	ASP	C-O	-5.62	1.18	1.24
1	B	429	GLY	C-O	-5.62	1.18	1.23
1	G	128	GLY	C-O	-5.62	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	482	ALA	CA-CB	-5.61	1.44	1.53
1	H	329	VAL	C-O	-5.61	1.18	1.24
1	D	482	ALA	CA-CB	-5.61	1.44	1.53
1	F	329	VAL	C-O	-5.61	1.18	1.24
1	A	478	HIS	C-O	-5.60	1.15	1.23
1	C	67	SER	C-O	-5.60	1.17	1.23
1	C	387	ALA	CA-CB	-5.60	1.45	1.53
1	G	18	LEU	C-O	-5.60	1.17	1.24
1	D	434	THR	N-CA	-5.60	1.39	1.46
1	D	305	SER	CA-C	-5.60	1.45	1.52
1	G	330	VAL	C-O	-5.60	1.17	1.24
1	H	482	ALA	CA-CB	-5.60	1.44	1.53
1	C	128	GLY	C-O	-5.59	1.17	1.23
1	F	79	GLU	C-O	-5.59	1.16	1.24
1	E	478	HIS	C-O	-5.59	1.15	1.23
1	G	482	ALA	CA-CB	-5.59	1.44	1.53
1	H	384	THR	C-O	-5.59	1.17	1.24
1	E	44	THR	C-O	-5.59	1.17	1.24
1	B	79	GLU	C-O	-5.59	1.16	1.24
1	D	44	THR	C-O	-5.59	1.17	1.24
1	H	434	THR	N-CA	-5.59	1.39	1.46
1	D	128	GLY	C-O	-5.58	1.17	1.23
1	B	329	VAL	C-O	-5.58	1.18	1.24
1	C	329	VAL	C-O	-5.58	1.18	1.24
1	C	330	VAL	C-O	-5.58	1.17	1.24
1	F	67	SER	C-O	-5.58	1.17	1.23
1	G	329	VAL	C-O	-5.58	1.18	1.24
1	F	305	SER	CA-C	-5.58	1.45	1.52
1	B	330	VAL	C-O	-5.58	1.17	1.24
1	C	303	ALA	CA-CB	-5.57	1.44	1.53
1	H	303	ALA	CA-CB	-5.57	1.44	1.53
1	C	478	HIS	C-O	-5.57	1.15	1.23
1	A	329	VAL	C-O	-5.57	1.18	1.24
1	A	384	THR	C-O	-5.57	1.17	1.24
1	B	67	SER	C-O	-5.57	1.17	1.23
1	C	367	ILE	C-O	-5.57	1.18	1.24
1	C	482	ALA	CA-CB	-5.57	1.44	1.53
1	F	84	ARG	C-O	-5.57	1.17	1.24
1	H	429	GLY	C-O	-5.57	1.18	1.23
1	D	384	THR	C-O	-5.57	1.17	1.24
1	G	384	THR	C-O	-5.57	1.17	1.24
1	A	44	THR	C-O	-5.56	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	128	GLY	C-O	-5.56	1.17	1.23
1	F	482	ALA	CA-CB	-5.56	1.44	1.53
1	B	84	ARG	C-O	-5.56	1.17	1.24
1	D	303	ALA	CA-CB	-5.56	1.44	1.53
1	E	330	VAL	C-O	-5.56	1.17	1.24
1	D	429	GLY	C-O	-5.55	1.18	1.23
1	F	384	THR	C-O	-5.55	1.17	1.24
1	A	128	GLY	C-O	-5.55	1.17	1.23
1	B	18	LEU	C-O	-5.55	1.17	1.24
1	G	130	ALA	CA-CB	-5.55	1.43	1.53
1	E	303	ALA	CA-CB	-5.55	1.44	1.53
1	F	330	VAL	C-O	-5.55	1.17	1.24
1	H	83	LEU	C-O	-5.54	1.17	1.24
1	C	384	THR	C-O	-5.54	1.17	1.24
1	H	44	THR	C-O	-5.54	1.17	1.24
1	A	303	ALA	CA-CB	-5.54	1.44	1.53
1	D	83	LEU	C-O	-5.54	1.17	1.24
1	G	461	ASP	C-O	-5.54	1.18	1.24
1	C	79	GLU	C-O	-5.54	1.17	1.24
1	D	329	VAL	C-O	-5.54	1.18	1.24
1	E	128	GLY	C-O	-5.54	1.17	1.23
1	B	44	THR	C-O	-5.53	1.17	1.24
1	E	83	LEU	C-O	-5.53	1.17	1.24
1	A	83	LEU	C-O	-5.53	1.17	1.24
1	B	384	THR	C-O	-5.53	1.17	1.24
1	C	130	ALA	CA-CB	-5.53	1.43	1.53
1	D	461	ASP	C-O	-5.53	1.18	1.24
1	G	303	ALA	CA-CB	-5.52	1.44	1.53
1	E	329	VAL	C-O	-5.52	1.18	1.24
1	A	330	VAL	C-O	-5.52	1.17	1.24
1	E	384	THR	C-O	-5.51	1.17	1.24
1	A	425	VAL	C-O	-5.50	1.18	1.24
1	H	57	ALA	C-O	-5.49	1.17	1.24
1	C	44	THR	C-O	-5.48	1.17	1.24
1	F	44	THR	C-O	-5.48	1.17	1.24
1	G	79	GLU	C-O	-5.48	1.17	1.24
1	B	303	ALA	CA-CB	-5.48	1.45	1.53
1	C	461	ASP	C-O	-5.48	1.18	1.24
1	F	57	ALA	C-O	-5.48	1.17	1.24
1	E	57	ALA	C-O	-5.47	1.17	1.24
1	F	461	ASP	C-O	-5.47	1.18	1.24
1	H	392	LYS	C-O	-5.47	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	330	VAL	C-O	-5.47	1.17	1.24
1	G	57	ALA	C-O	-5.47	1.17	1.24
1	A	36	ASN	C-O	-5.46	1.17	1.24
1	F	18	LEU	C-O	-5.46	1.17	1.24
1	F	303	ALA	CA-CB	-5.46	1.45	1.53
1	G	44	THR	C-O	-5.46	1.17	1.24
1	C	57	ALA	C-O	-5.45	1.17	1.24
1	D	73	MET	CA-C	-5.45	1.46	1.52
1	F	73	MET	CA-C	-5.45	1.46	1.52
1	B	57	ALA	C-O	-5.45	1.17	1.24
1	E	36	ASN	C-O	-5.45	1.17	1.24
1	A	47	PRO	C-O	-5.44	1.18	1.23
1	C	358	ASN	CA-CB	-5.44	1.44	1.53
1	A	73	MET	CA-C	-5.44	1.46	1.52
1	B	73	MET	CA-C	-5.44	1.46	1.52
1	H	54	VAL	C-O	-5.44	1.17	1.24
1	D	357	ARG	C-O	-5.44	1.17	1.24
1	B	461	ASP	C-O	-5.43	1.18	1.24
1	E	73	MET	CA-C	-5.43	1.46	1.52
1	H	73	MET	CA-C	-5.43	1.46	1.52
1	A	57	ALA	C-O	-5.43	1.17	1.24
1	A	357	ARG	C-O	-5.43	1.17	1.24
1	D	57	ALA	C-O	-5.43	1.17	1.24
1	H	330	VAL	C-O	-5.43	1.17	1.24
1	D	54	VAL	C-O	-5.43	1.17	1.24
1	C	73	MET	CA-C	-5.42	1.46	1.52
1	F	123	LEU	C-O	-5.42	1.17	1.24
1	E	357	ARG	C-O	-5.42	1.17	1.24
1	G	358	ASN	CA-CB	-5.42	1.44	1.53
1	B	123	LEU	C-O	-5.42	1.17	1.24
1	E	130	ALA	CA-CB	-5.41	1.43	1.53
1	C	426	TYR	CA-CB	-5.41	1.45	1.53
1	B	431	SER	C-O	-5.41	1.17	1.23
1	F	346	LYS	C-O	-5.41	1.16	1.24
1	F	340	MET	C-O	-5.40	1.17	1.23
1	H	431	SER	C-O	-5.40	1.17	1.23
1	A	123	LEU	C-O	-5.40	1.17	1.24
1	H	77	ALA	C-O	-5.40	1.17	1.24
1	D	129	TRP	C-O	-5.40	1.16	1.24
1	E	123	LEU	C-O	-5.40	1.17	1.24
1	E	54	VAL	C-O	-5.40	1.17	1.24
1	A	211	ALA	CA-CB	-5.39	1.43	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	54	VAL	C-O	-5.39	1.17	1.24
1	E	47	PRO	C-O	-5.39	1.18	1.23
1	E	211	ALA	CA-CB	-5.38	1.43	1.53
1	A	130	ALA	CA-CB	-5.38	1.43	1.53
1	A	431	SER	C-O	-5.38	1.17	1.23
1	B	357	ARG	C-O	-5.38	1.17	1.24
1	C	123	LEU	C-O	-5.38	1.17	1.24
1	G	227	THR	CA-C	5.38	1.57	1.52
1	C	81	ILE	C-O	-5.38	1.17	1.24
1	G	73	MET	CA-C	-5.38	1.46	1.52
1	F	357	ARG	C-O	-5.38	1.17	1.24
1	E	482	ALA	CA-C	-5.38	1.46	1.52
1	D	431	SER	C-O	-5.38	1.17	1.23
1	G	54	VAL	C-O	-5.38	1.17	1.24
1	H	467	GLY	C-O	-5.38	1.17	1.24
1	F	431	SER	C-O	-5.37	1.17	1.23
1	H	430	ALA	CA-CB	-5.37	1.44	1.53
1	A	426	TYR	CA-C	-5.37	1.46	1.52
1	B	54	VAL	C-O	-5.37	1.17	1.24
1	F	482	ALA	CA-C	-5.37	1.46	1.52
1	G	414	ILE	C-O	-5.37	1.17	1.24
1	A	54	VAL	C-O	-5.37	1.17	1.24
1	F	54	VAL	C-O	-5.37	1.17	1.24
1	H	346	LYS	C-O	-5.37	1.17	1.24
1	B	346	LYS	C-O	-5.37	1.17	1.24
1	C	430	ALA	CA-CB	-5.37	1.44	1.53
1	H	482	ALA	CA-C	-5.37	1.46	1.52
1	A	430	ALA	CA-CB	-5.36	1.44	1.53
1	B	430	ALA	CA-CB	-5.36	1.44	1.53
1	D	467	GLY	C-O	-5.36	1.17	1.24
1	F	440	ALA	C-O	-5.36	1.17	1.24
1	H	129	TRP	C-O	-5.36	1.16	1.24
1	B	340	MET	C-O	-5.36	1.17	1.23
1	F	430	ALA	CA-CB	-5.36	1.44	1.53
1	C	482	ALA	CA-C	-5.36	1.46	1.52
1	E	129	TRP	C-O	-5.36	1.17	1.24
1	D	430	ALA	CA-CB	-5.36	1.44	1.53
1	G	123	LEU	C-O	-5.36	1.17	1.24
1	A	129	TRP	C-O	-5.35	1.17	1.24
1	E	62	ALA	C-N	-5.35	1.26	1.33
1	A	482	ALA	CA-C	-5.35	1.46	1.52
1	B	211	ALA	CA-CB	-5.35	1.43	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	77	ALA	C-O	-5.35	1.17	1.24
1	C	211	ALA	CA-CB	-5.34	1.43	1.53
1	D	211	ALA	CA-CB	-5.34	1.43	1.53
1	A	62	ALA	C-N	-5.34	1.27	1.33
1	C	77	ALA	C-O	-5.34	1.17	1.24
1	G	170	PHE	C-O	-5.34	1.18	1.24
1	A	77	ALA	C-O	-5.34	1.17	1.24
1	C	314	TYR	C-O	-5.34	1.18	1.24
1	E	77	ALA	C-O	-5.34	1.17	1.24
1	F	211	ALA	CA-CB	-5.34	1.43	1.53
1	D	482	ALA	CA-C	-5.34	1.46	1.52
1	G	211	ALA	CA-CB	-5.34	1.43	1.53
1	G	314	TYR	C-O	-5.34	1.18	1.24
1	H	357	ARG	C-O	-5.34	1.17	1.24
1	G	340	MET	C-O	-5.33	1.17	1.23
1	G	482	ALA	CA-C	-5.33	1.46	1.52
1	H	211	ALA	CA-CB	-5.33	1.43	1.53
1	C	340	MET	C-O	-5.33	1.17	1.23
1	A	346	LYS	C-O	-5.33	1.17	1.24
1	E	414	ILE	C-O	-5.33	1.17	1.24
1	E	430	ALA	CA-CB	-5.33	1.44	1.53
1	A	414	ILE	C-O	-5.33	1.17	1.24
1	F	77	ALA	C-O	-5.33	1.17	1.24
1	H	123	LEU	C-O	-5.33	1.18	1.24
1	A	373	ALA	CA-C	-5.33	1.46	1.52
1	G	42	ILE	C-O	-5.33	1.18	1.24
1	H	127	ALA	CA-CB	-5.33	1.44	1.53
1	C	431	SER	C-O	-5.32	1.17	1.23
1	B	77	ALA	C-O	-5.32	1.17	1.24
1	C	456	THR	C-O	-5.32	1.18	1.23
1	D	127	ALA	CA-CB	-5.32	1.44	1.53
1	E	456	THR	C-O	-5.32	1.18	1.23
1	B	151	ARG	C-O	-5.32	1.17	1.24
1	B	467	GLY	C-O	-5.32	1.17	1.24
1	C	42	ILE	C-O	-5.32	1.18	1.24
1	D	346	LYS	C-O	-5.32	1.17	1.24
1	G	81	ILE	C-O	-5.32	1.18	1.24
1	A	340	MET	C-O	-5.31	1.17	1.23
1	A	370	GLY	C-O	-5.31	1.16	1.23
1	D	314	TYR	C-O	-5.31	1.18	1.24
1	G	430	ALA	CA-CB	-5.31	1.44	1.53
1	H	61	ALA	C-O	-5.31	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	314	TYR	C-O	-5.31	1.18	1.24
1	A	467	GLY	C-O	-5.31	1.17	1.24
1	E	314	TYR	C-O	-5.31	1.18	1.24
1	G	467	GLY	C-O	-5.31	1.17	1.24
1	A	456	THR	C-O	-5.31	1.18	1.23
1	B	61	ALA	C-O	-5.31	1.17	1.24
1	C	127	ALA	CA-CB	-5.31	1.44	1.53
1	C	467	GLY	C-O	-5.31	1.17	1.24
1	E	467	GLY	C-O	-5.31	1.17	1.24
1	G	431	SER	C-O	-5.31	1.17	1.23
1	G	115	GLU	CA-C	-5.30	1.45	1.52
1	G	39	THR	CA-C	-5.30	1.46	1.53
1	G	127	ALA	CA-CB	-5.30	1.44	1.53
1	A	127	ALA	CA-CB	-5.30	1.44	1.53
1	E	346	LYS	C-O	-5.30	1.17	1.24
1	E	431	SER	C-O	-5.30	1.17	1.23
1	F	61	ALA	C-O	-5.30	1.17	1.24
1	D	123	LEU	C-O	-5.30	1.18	1.24
1	F	467	GLY	C-O	-5.30	1.17	1.24
1	C	346	LYS	C-O	-5.30	1.17	1.24
1	A	61	ALA	C-O	-5.29	1.17	1.24
1	D	340	MET	C-O	-5.29	1.17	1.23
1	B	440	ALA	C-O	-5.29	1.17	1.24
1	B	81	ILE	C-O	-5.29	1.17	1.24
1	B	414	ILE	C-O	-5.29	1.17	1.24
1	E	61	ALA	CA-C	-5.29	1.45	1.52
1	E	425	VAL	C-O	-5.29	1.18	1.24
1	F	115	GLU	CA-C	-5.29	1.45	1.52
1	G	77	ALA	C-O	-5.28	1.17	1.24
1	G	456	THR	C-O	-5.28	1.18	1.23
1	D	61	ALA	C-O	-5.28	1.17	1.24
1	G	61	ALA	CA-C	-5.28	1.45	1.52
1	C	61	ALA	C-O	-5.28	1.17	1.24
1	G	140	LEU	N-CA	-5.28	1.39	1.46
1	A	314	TYR	C-O	-5.28	1.18	1.24
1	C	61	ALA	CA-C	-5.28	1.45	1.52
1	E	127	ALA	CA-CB	-5.28	1.44	1.53
1	H	427	GLY	C-O	-5.28	1.16	1.23
1	B	456	THR	C-O	-5.27	1.18	1.23
1	F	17	MET	C-O	-5.27	1.17	1.23
1	F	151	ARG	C-O	-5.27	1.17	1.24
1	C	115	GLU	CA-C	-5.27	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	81	ILE	C-O	-5.27	1.17	1.24
1	E	265	SER	C-O	-5.27	1.17	1.24
1	E	340	MET	C-O	-5.27	1.17	1.23
1	A	440	ALA	C-O	-5.27	1.17	1.24
1	F	456	THR	C-O	-5.27	1.18	1.23
1	H	340	MET	C-O	-5.27	1.17	1.23
1	A	60	SER	C-O	-5.26	1.17	1.24
1	C	39	THR	CA-C	-5.26	1.46	1.53
1	C	60	SER	C-O	-5.26	1.17	1.24
1	G	346	LYS	C-O	-5.26	1.17	1.24
1	E	440	ALA	C-O	-5.26	1.17	1.24
1	H	60	SER	C-O	-5.26	1.17	1.24
1	F	61	ALA	CA-C	-5.26	1.45	1.52
1	F	414	ILE	C-O	-5.26	1.17	1.24
1	A	115	GLU	CA-C	-5.25	1.46	1.52
1	F	367	ILE	C-O	-5.25	1.18	1.24
1	B	314	TYR	C-O	-5.25	1.18	1.24
1	D	456	THR	C-O	-5.25	1.18	1.23
1	B	60	SER	C-O	-5.25	1.17	1.24
1	E	23	TRP	CA-C	-5.25	1.46	1.52
1	A	61	ALA	CA-C	-5.24	1.45	1.52
1	F	60	SER	C-O	-5.24	1.17	1.24
1	A	81	ILE	C-O	-5.24	1.18	1.24
1	E	81	ILE	C-O	-5.24	1.18	1.24
1	F	392	LYS	C-O	-5.24	1.17	1.23
1	F	482	ALA	C-O	-5.24	1.18	1.24
1	B	367	ILE	C-O	-5.24	1.18	1.24
1	D	265	SER	C-O	-5.24	1.17	1.24
1	F	314	TYR	C-O	-5.24	1.18	1.24
1	D	60	SER	C-O	-5.23	1.17	1.24
1	D	115	GLU	CA-C	-5.23	1.46	1.52
1	E	61	ALA	C-O	-5.23	1.17	1.24
1	F	81	ILE	C-O	-5.23	1.18	1.24
1	H	405	VAL	C-O	-5.23	1.18	1.24
1	H	81	ILE	C-O	-5.23	1.18	1.24
1	E	60	SER	C-O	-5.23	1.17	1.24
1	H	119	SER	CA-C	-5.23	1.46	1.52
1	H	115	GLU	CA-C	-5.23	1.46	1.52
1	A	265	SER	C-O	-5.22	1.17	1.24
1	B	115	GLU	CA-C	-5.22	1.46	1.52
1	D	61	ALA	CA-C	-5.22	1.45	1.52
1	G	265	SER	C-O	-5.22	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	119	SER	CA-C	-5.22	1.46	1.52
1	H	23	TRP	CA-C	-5.22	1.46	1.52
1	E	482	ALA	C-O	-5.22	1.18	1.24
1	C	265	SER	C-O	-5.22	1.17	1.24
1	A	482	ALA	C-O	-5.22	1.18	1.24
1	B	265	SER	C-O	-5.21	1.17	1.24
1	G	60	SER	C-O	-5.21	1.17	1.24
1	H	61	ALA	CA-C	-5.21	1.45	1.52
1	E	115	GLU	CA-C	-5.21	1.46	1.52
1	H	59	GLU	C-O	-5.21	1.17	1.24
1	H	456	THR	C-O	-5.21	1.18	1.23
1	H	265	SER	C-O	-5.21	1.17	1.24
1	H	383	PRO	C-O	-5.21	1.16	1.23
1	C	47	PRO	C-O	-5.21	1.18	1.23
1	C	482	ALA	C-O	-5.21	1.18	1.24
1	G	61	ALA	C-O	-5.21	1.17	1.24
1	A	86	ALA	C-O	-5.20	1.17	1.24
1	A	373	ALA	CA-CB	-5.20	1.42	1.53
1	B	61	ALA	CA-C	-5.20	1.45	1.52
1	E	367	ILE	C-O	-5.20	1.18	1.24
1	F	47	PRO	C-O	-5.20	1.18	1.23
1	A	23	TRP	CA-C	-5.20	1.46	1.52
1	A	383	PRO	C-O	-5.19	1.16	1.23
1	G	47	PRO	C-O	-5.19	1.18	1.23
1	D	23	TRP	CA-C	-5.19	1.46	1.52
1	H	47	PRO	C-O	-5.19	1.18	1.23
1	B	47	PRO	C-O	-5.19	1.18	1.23
1	E	59	GLU	C-O	-5.19	1.17	1.24
1	B	319	GLN	C-O	-5.18	1.18	1.24
1	F	265	SER	C-O	-5.18	1.17	1.24
1	A	119	SER	CA-C	-5.18	1.46	1.52
1	D	405	VAL	C-O	-5.18	1.18	1.24
1	B	23	TRP	CA-C	-5.18	1.46	1.52
1	D	436	ASP	C-O	-5.18	1.17	1.24
1	E	86	ALA	C-O	-5.18	1.17	1.24
1	F	23	TRP	CA-C	-5.18	1.46	1.52
1	G	86	ALA	C-O	-5.18	1.17	1.24
1	C	429	GLY	C-O	-5.18	1.18	1.23
1	D	482	ALA	C-O	-5.18	1.18	1.24
1	E	436	ASP	C-O	-5.18	1.17	1.23
1	F	59	GLU	C-O	-5.18	1.17	1.24
1	F	383	PRO	C-O	-5.18	1.16	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	429	GLY	C-O	-5.17	1.18	1.23
1	H	436	ASP	C-O	-5.17	1.17	1.24
1	B	383	PRO	C-O	-5.17	1.16	1.23
1	C	86	ALA	C-O	-5.17	1.17	1.24
1	D	383	PRO	C-O	-5.17	1.16	1.23
1	G	367	ILE	C-O	-5.17	1.18	1.24
1	G	482	ALA	C-O	-5.17	1.18	1.24
1	H	482	ALA	C-O	-5.17	1.18	1.24
1	F	429	GLY	C-O	-5.17	1.18	1.23
1	F	434	THR	C-O	-5.17	1.17	1.24
1	G	441	LEU	C-O	-5.17	1.17	1.24
1	C	441	LEU	C-O	-5.17	1.17	1.24
1	E	383	PRO	C-O	-5.17	1.16	1.23
1	C	80	ARG	C-O	-5.16	1.17	1.24
1	D	367	ILE	C-O	-5.16	1.18	1.24
1	G	319	GLN	C-O	-5.16	1.18	1.24
1	G	80	ARG	C-O	-5.16	1.17	1.24
1	A	393	ASP	N-CA	-5.16	1.40	1.46
1	B	59	GLU	C-O	-5.16	1.17	1.24
1	C	59	GLU	C-O	-5.16	1.17	1.24
1	F	131	THR	C-O	-5.16	1.17	1.24
1	G	59	GLU	C-O	-5.16	1.17	1.24
1	H	367	ILE	C-O	-5.16	1.18	1.24
1	F	35	TYR	C-O	-5.15	1.17	1.23
1	A	59	GLU	C-O	-5.15	1.17	1.24
1	C	383	PRO	C-O	-5.15	1.16	1.23
1	A	436	ASP	C-O	-5.15	1.17	1.23
1	B	35	TYR	C-O	-5.15	1.17	1.23
1	B	86	ALA	C-O	-5.15	1.17	1.24
1	C	23	TRP	C-O	-5.15	1.17	1.24
1	G	405	VAL	C-O	-5.15	1.18	1.24
1	B	434	THR	C-O	-5.14	1.17	1.24
1	C	119	SER	CA-C	-5.14	1.46	1.52
1	H	86	ALA	C-O	-5.14	1.17	1.24
1	H	414	ILE	C-O	-5.14	1.17	1.24
1	A	434	THR	C-O	-5.14	1.17	1.24
1	D	59	GLU	C-O	-5.14	1.17	1.24
1	C	319	GLN	C-O	-5.14	1.18	1.24
1	D	434	THR	CA-C	-5.14	1.46	1.52
1	F	319	GLN	C-O	-5.14	1.18	1.24
1	F	405	VAL	C-O	-5.14	1.18	1.24
1	G	434	THR	CA-C	-5.14	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	131	THR	C-O	-5.13	1.17	1.24
1	D	86	ALA	C-O	-5.13	1.17	1.24
1	D	47	PRO	C-O	-5.13	1.18	1.23
1	A	319	GLN	C-O	-5.13	1.18	1.24
1	C	358	ASN	CB-CG	-5.13	1.39	1.52
1	H	434	THR	CA-C	-5.13	1.46	1.52
1	G	23	TRP	C-O	-5.13	1.17	1.24
1	H	50	ASP	CA-C	-5.13	1.48	1.53
1	E	119	SER	CA-C	-5.13	1.46	1.52
1	C	434	THR	CA-C	-5.12	1.46	1.52
1	F	387	ALA	CA-CB	-5.12	1.46	1.53
1	F	86	ALA	C-O	-5.12	1.17	1.24
1	C	405	VAL	C-O	-5.12	1.18	1.24
1	H	415	ALA	CA-CB	-5.12	1.45	1.53
1	G	119	SER	CA-C	-5.12	1.46	1.52
1	G	385	ILE	C-O	-5.12	1.18	1.24
1	D	414	ILE	C-O	-5.12	1.17	1.24
1	F	436	ASP	C-O	-5.12	1.17	1.23
1	G	23	TRP	CA-C	-5.12	1.46	1.52
1	G	358	ASN	CB-CG	-5.12	1.39	1.52
1	C	414	ILE	C-O	-5.11	1.17	1.24
1	F	36	ASN	C-O	-5.11	1.18	1.24
1	A	50	ASP	CA-C	-5.11	1.48	1.53
1	B	387	ALA	CA-CB	-5.11	1.46	1.53
1	C	385	ILE	C-O	-5.11	1.18	1.24
1	C	23	TRP	CA-C	-5.11	1.46	1.52
1	E	319	GLN	C-O	-5.11	1.18	1.24
1	E	50	ASP	CA-C	-5.10	1.48	1.53
1	B	127	ALA	CA-CB	-5.10	1.44	1.53
1	H	444	ASN	C-O	-5.10	1.18	1.24
1	B	405	VAL	C-O	-5.10	1.18	1.24
1	G	50	ASP	CA-C	-5.10	1.48	1.53
1	A	385	ILE	C-O	-5.10	1.18	1.24
1	D	319	GLN	C-O	-5.10	1.18	1.24
1	F	50	ASP	CA-C	-5.10	1.48	1.53
1	G	383	PRO	C-O	-5.10	1.17	1.23
1	A	387	ALA	CA-CB	-5.09	1.46	1.53
1	A	415	ALA	CA-CB	-5.09	1.45	1.53
1	E	405	VAL	C-O	-5.09	1.18	1.24
1	D	415	ALA	CA-CB	-5.09	1.45	1.53
1	E	385	ILE	C-O	-5.09	1.18	1.24
1	E	415	ALA	CA-CB	-5.09	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	127	ALA	CA-CB	-5.09	1.44	1.53
1	G	109	ILE	C-O	-5.09	1.18	1.24
1	G	148	VAL	C-O	-5.09	1.18	1.24
1	A	405	VAL	C-O	-5.09	1.18	1.24
1	E	434	THR	C-O	-5.08	1.17	1.24
1	C	357	ARG	C-O	-5.08	1.17	1.24
1	D	50	ASP	CA-C	-5.08	1.48	1.53
1	B	50	ASP	CA-C	-5.07	1.48	1.53
1	F	415	ALA	CA-CB	-5.07	1.45	1.53
1	C	109	ILE	C-O	-5.07	1.18	1.24
1	F	385	ILE	C-O	-5.07	1.18	1.24
1	H	319	GLN	C-O	-5.07	1.18	1.24
1	D	444	ASN	C-O	-5.06	1.18	1.24
1	H	385	ILE	C-O	-5.06	1.18	1.24
1	A	444	ASN	C-O	-5.06	1.18	1.24
1	C	50	ASP	CA-C	-5.06	1.48	1.53
1	D	385	ILE	C-O	-5.06	1.18	1.24
1	B	23	TRP	C-O	-5.06	1.17	1.24
1	E	438	SER	C-O	-5.06	1.18	1.24
1	B	415	ALA	CA-CB	-5.06	1.45	1.53
1	C	435	ASN	N-CA	-5.06	1.41	1.46
1	B	444	ASN	C-O	-5.05	1.18	1.24
1	F	444	ASN	C-O	-5.05	1.18	1.24
1	B	385	ILE	C-O	-5.05	1.18	1.24
1	B	436	ASP	C-O	-5.05	1.17	1.23
1	G	444	ASN	C-O	-5.05	1.18	1.24
1	A	23	TRP	C-O	-5.04	1.17	1.24
1	G	435	ASN	N-CA	-5.04	1.41	1.46
1	F	222	THR	C-O	-5.04	1.17	1.23
1	H	438	SER	C-O	-5.04	1.18	1.24
1	D	364	ALA	CA-CB	-5.04	1.45	1.53
1	F	23	TRP	C-O	-5.04	1.17	1.24
1	C	444	ASN	C-O	-5.04	1.18	1.24
1	G	357	ARG	C-O	-5.04	1.17	1.24
1	C	438	SER	C-O	-5.03	1.18	1.24
1	E	387	ALA	CA-CB	-5.03	1.46	1.53
1	C	442	ARG	C-O	-5.03	1.18	1.24
1	D	483	ILE	C-O	-5.03	1.17	1.24
1	E	364	ALA	CA-CB	-5.03	1.45	1.53
1	H	23	TRP	C-O	-5.02	1.17	1.24
1	E	23	TRP	C-O	-5.02	1.17	1.24
1	E	481	ALA	C-O	-5.02	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	444	ASN	C-O	-5.02	1.18	1.24
1	B	222	THR	C-O	-5.02	1.17	1.23
1	F	364	ALA	CA-CB	-5.02	1.45	1.53
1	D	438	SER	C-O	-5.01	1.18	1.24
1	G	481	ALA	C-O	-5.01	1.17	1.24
1	H	483	ILE	C-O	-5.01	1.17	1.24
1	B	364	ALA	CA-CB	-5.01	1.45	1.53
1	C	144	LEU	CA-C	-5.01	1.46	1.52
1	C	364	ALA	CA-CB	-5.01	1.45	1.53
1	D	17	MET	C-O	-5.01	1.17	1.23
1	F	481	ALA	C-O	-5.01	1.17	1.24
1	D	23	TRP	C-O	-5.00	1.17	1.24
1	A	364	ALA	CA-CB	-5.00	1.45	1.53
1	C	481	ALA	C-O	-5.00	1.17	1.24

All (644) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	428	LEU	N-CA-C	14.78	127.08	110.97
1	H	269	GLY	N-CA-C	13.14	126.79	112.33
1	D	269	GLY	N-CA-C	13.14	126.78	112.33
1	E	269	GLY	N-CA-C	13.11	126.75	112.33
1	A	269	GLY	N-CA-C	13.11	126.75	112.33
1	C	269	GLY	N-CA-C	13.11	126.75	112.33
1	G	269	GLY	N-CA-C	13.10	126.75	112.33
1	D	396	LEU	N-CA-C	-12.37	97.89	113.23
1	D	428	LEU	N-CA-C	12.34	124.28	111.07
1	A	428	LEU	N-CA-C	10.74	124.90	111.69
1	B	395	ARG	N-CA-C	10.41	126.41	112.25
1	B	269	GLY	N-CA-C	10.30	126.05	112.25
1	F	396	LEU	N-CA-C	-10.28	100.76	113.20
1	H	443	ILE	N-CA-C	-10.01	98.58	111.09
1	D	443	ILE	N-CA-C	-10.00	98.59	111.09
1	B	428	LEU	N-CA-C	9.90	123.86	111.69
1	B	389	ARG	N-CA-C	-9.71	97.71	110.43
1	F	428	LEU	N-CA-C	9.63	121.72	111.03
1	C	391	LYS	N-CA-C	9.52	124.60	111.17
1	A	396	LEU	N-CA-C	-9.52	101.35	113.16
1	E	63	ALA	N-CA-C	9.38	122.68	111.33
1	A	63	ALA	N-CA-C	9.35	122.64	111.33
1	B	130	ALA	N-CA-C	-9.27	99.57	112.45
1	F	130	ALA	N-CA-C	-9.27	99.57	112.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	428	LEU	N-CA-C	9.23	124.99	112.90
1	D	89	LEU	N-CA-C	-9.13	102.28	113.41
1	H	89	LEU	N-CA-C	-9.10	102.30	113.41
1	E	125	TYR	N-CA-C	9.03	123.31	111.75
1	C	125	TYR	N-CA-C	9.02	123.30	111.75
1	A	125	TYR	N-CA-C	9.02	123.29	111.75
1	D	125	TYR	N-CA-C	9.00	123.27	111.75
1	B	125	TYR	N-CA-C	8.99	123.26	111.75
1	H	125	TYR	N-CA-C	8.99	123.25	111.75
1	G	125	TYR	N-CA-C	8.98	123.25	111.75
1	F	125	TYR	N-CA-C	8.97	123.23	111.75
1	F	269	GLY	N-CA-C	8.80	122.01	112.33
1	E	357	ARG	N-CA-C	8.70	120.76	111.28
1	A	357	ARG	N-CA-C	8.69	120.75	111.28
1	B	357	ARG	N-CA-C	8.67	120.73	111.28
1	D	357	ARG	N-CA-C	8.67	120.73	111.28
1	H	357	ARG	N-CA-C	8.66	120.72	111.28
1	F	357	ARG	N-CA-C	8.66	120.72	111.28
1	E	396	LEU	N-CA-C	-8.61	102.92	113.50
1	C	394	ILE	N-CA-C	-8.56	95.05	107.98
1	A	175	ALA	N-CA-C	8.51	120.64	111.36
1	E	175	ALA	N-CA-C	8.50	120.63	111.36
1	G	142	LEU	C-N-CD	8.49	139.29	120.60
1	E	139	ASP	CA-C-N	-8.41	107.14	121.94
1	E	139	ASP	C-N-CA	-8.41	107.14	121.94
1	B	54	VAL	N-CA-C	-8.39	100.53	112.35
1	D	142	LEU	C-N-CD	-8.38	102.15	120.60
1	A	54	VAL	N-CA-C	-8.37	100.54	112.35
1	D	54	VAL	N-CA-C	-8.37	100.55	112.35
1	F	54	VAL	N-CA-C	-8.37	100.55	112.35
1	G	54	VAL	N-CA-C	-8.37	100.56	112.35
1	H	54	VAL	N-CA-C	-8.36	100.56	112.35
1	E	54	VAL	N-CA-C	-8.36	100.56	112.35
1	C	54	VAL	N-CA-C	-8.35	100.57	112.35
1	G	317	VAL	N-CA-C	8.30	120.08	110.62
1	C	317	VAL	N-CA-C	8.29	120.07	110.62
1	A	317	VAL	N-CA-C	8.28	120.06	110.62
1	E	317	VAL	N-CA-C	8.28	120.06	110.62
1	H	317	VAL	N-CA-C	8.27	120.05	110.62
1	D	317	VAL	N-CA-C	8.27	120.04	110.62
1	B	317	VAL	N-CA-C	8.23	120.00	110.62
1	F	317	VAL	N-CA-C	8.23	120.00	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	391	LYS	N-CA-C	8.21	122.58	111.24
1	G	142	LEU	N-CA-C	8.21	127.95	109.81
1	G	144	LEU	CA-C-N	-8.17	111.97	120.38
1	G	144	LEU	C-N-CA	-8.17	111.97	120.38
1	D	484	GLU	N-CA-C	8.04	122.86	112.89
1	H	484	GLU	N-CA-C	8.01	122.82	112.89
1	E	302	THR	N-CA-C	7.99	122.40	113.21
1	D	302	THR	N-CA-C	7.96	122.36	113.21
1	H	302	THR	N-CA-C	7.95	122.36	113.21
1	A	302	THR	N-CA-C	7.93	122.33	113.21
1	G	302	THR	N-CA-C	7.93	122.33	113.21
1	B	302	THR	N-CA-C	7.91	122.31	113.21
1	C	302	THR	N-CA-C	7.91	122.31	113.21
1	B	415	ALA	N-CA-C	7.91	120.80	111.71
1	D	415	ALA	N-CA-C	7.90	120.79	111.71
1	F	302	THR	N-CA-C	7.90	122.29	113.21
1	A	415	ALA	N-CA-C	7.89	120.78	111.71
1	B	148	VAL	N-CA-CB	7.89	124.25	111.23
1	F	415	ALA	N-CA-C	7.89	120.78	111.71
1	E	415	ALA	N-CA-C	7.88	120.78	111.71
1	G	357	ARG	N-CA-C	7.87	120.77	111.71
1	C	357	ARG	N-CA-C	7.86	120.75	111.71
1	H	415	ALA	N-CA-C	7.86	120.75	111.71
1	C	441	LEU	CA-C-N	7.81	133.94	120.58
1	C	441	LEU	C-N-CA	7.81	133.94	120.58
1	G	441	LEU	CA-C-N	7.81	133.93	120.58
1	G	441	LEU	C-N-CA	7.81	133.93	120.58
1	C	146	PRO	CA-C-N	-7.77	110.85	123.05
1	C	146	PRO	C-N-CA	-7.77	110.85	123.05
1	C	391	LYS	N-CA-CB	-7.68	100.04	111.71
1	B	36	ASN	N-CA-C	-7.60	99.82	110.31
1	C	142	LEU	N-CA-C	7.54	126.48	109.81
1	H	139	ASP	N-CA-C	-7.51	99.09	110.14
1	E	205	ALA	N-CA-C	7.49	120.39	111.33
1	F	205	ALA	N-CA-C	7.47	120.36	111.33
1	G	205	ALA	N-CA-C	7.46	120.35	111.33
1	A	205	ALA	N-CA-C	7.45	120.34	111.33
1	C	205	ALA	N-CA-C	7.45	120.35	111.33
1	H	205	ALA	N-CA-C	7.45	120.34	111.33
1	D	205	ALA	N-CA-C	7.45	120.34	111.33
1	F	260	SER	N-CA-C	7.45	121.95	113.01
1	B	205	ALA	N-CA-C	7.44	120.34	111.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	260	SER	N-CA-C	7.44	121.94	113.01
1	H	260	SER	N-CA-C	7.44	121.94	113.01
1	A	260	SER	N-CA-C	7.43	121.93	113.01
1	E	371	THR	N-CA-C	7.43	123.38	113.72
1	E	260	SER	N-CA-C	7.43	121.92	113.01
1	D	260	SER	N-CA-C	7.42	121.91	113.01
1	G	260	SER	N-CA-C	7.42	121.91	113.01
1	C	260	SER	N-CA-C	7.40	121.89	113.01
1	E	147	GLU	CB-CA-C	-7.40	98.87	110.04
1	A	139	ASP	N-CA-C	-7.39	99.52	110.46
1	G	195	GLU	N-CA-C	-7.38	104.42	113.50
1	F	195	GLU	N-CA-C	-7.37	104.43	113.50
1	D	195	GLU	N-CA-C	-7.36	104.45	113.50
1	B	195	GLU	N-CA-C	-7.36	104.45	113.50
1	C	195	GLU	N-CA-C	-7.36	104.45	113.50
1	A	195	GLU	N-CA-C	-7.35	104.46	113.50
1	E	195	GLU	N-CA-C	-7.34	104.47	113.50
1	H	195	GLU	N-CA-C	-7.33	104.48	113.50
1	H	392	LYS	N-CA-C	7.31	122.24	109.96
1	B	89	LEU	N-CA-C	-7.27	102.35	112.45
1	F	89	LEU	N-CA-C	-7.27	102.35	112.45
1	E	29	GLY	N-CA-C	-7.26	102.42	114.48
1	A	29	GLY	N-CA-C	-7.24	102.46	114.48
1	H	237	LYS	N-CA-C	7.18	122.06	113.16
1	C	237	LYS	N-CA-C	7.17	122.05	113.16
1	H	393	ASP	N-CA-C	-7.16	95.92	108.23
1	G	237	LYS	N-CA-C	7.16	122.03	113.16
1	D	237	LYS	N-CA-C	7.15	122.03	113.16
1	F	237	LYS	N-CA-C	7.15	122.02	113.16
1	A	237	LYS	N-CA-C	7.13	122.00	113.16
1	B	237	LYS	N-CA-C	7.13	122.00	113.16
1	G	48	ASP	CA-C-N	7.13	127.11	120.34
1	G	48	ASP	C-N-CA	7.13	127.11	120.34
1	E	237	LYS	N-CA-C	7.12	121.99	113.16
1	C	48	ASP	CA-C-N	7.07	127.06	120.34
1	C	48	ASP	C-N-CA	7.07	127.06	120.34
1	F	48	ASP	CA-C-N	7.05	127.04	120.34
1	F	48	ASP	C-N-CA	7.05	127.04	120.34
1	C	110	TYR	N-CA-C	7.05	119.81	111.71
1	H	48	ASP	CA-C-N	7.04	127.03	120.34
1	H	48	ASP	C-N-CA	7.04	127.03	120.34
1	A	48	ASP	CA-C-N	7.02	127.01	120.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	ASP	C-N-CA	7.02	127.01	120.34
1	D	48	ASP	CA-C-N	7.02	127.00	120.34
1	D	48	ASP	C-N-CA	7.02	127.00	120.34
1	B	48	ASP	CA-C-N	7.01	127.00	120.34
1	B	48	ASP	C-N-CA	7.01	127.00	120.34
1	G	110	TYR	N-CA-C	7.00	119.76	111.71
1	E	48	ASP	CA-C-N	7.00	126.99	120.34
1	E	48	ASP	C-N-CA	7.00	126.99	120.34
1	C	428	LEU	N-CA-C	6.96	119.89	111.40
1	B	146	PRO	CB-CA-C	-6.92	100.14	111.56
1	E	479	GLY	N-CA-C	6.92	124.12	110.77
1	D	479	GLY	N-CA-C	6.91	124.11	110.77
1	G	281	ASP	CA-C-N	6.91	126.16	118.97
1	G	281	ASP	C-N-CA	6.91	126.16	118.97
1	C	479	GLY	N-CA-C	6.90	124.09	110.77
1	A	479	GLY	N-CA-C	6.90	124.08	110.77
1	G	479	GLY	N-CA-C	6.90	124.08	110.77
1	B	479	GLY	N-CA-C	6.89	124.08	110.77
1	F	479	GLY	N-CA-C	6.89	124.07	110.77
1	H	479	GLY	N-CA-C	6.89	124.07	110.77
1	B	396	LEU	N-CA-C	-6.86	104.03	112.88
1	H	43	LEU	N-CA-C	-6.79	104.63	113.12
1	A	197	THR	CB-CA-C	-6.77	102.22	110.81
1	C	43	LEU	N-CA-C	-6.76	104.67	113.12
1	D	43	LEU	N-CA-C	-6.76	104.67	113.12
1	D	197	THR	CB-CA-C	-6.76	102.22	110.81
1	G	43	LEU	N-CA-C	-6.76	104.67	113.12
1	B	197	THR	CB-CA-C	-6.76	102.23	110.81
1	A	43	LEU	N-CA-C	-6.75	104.68	113.12
1	E	43	LEU	N-CA-C	-6.75	104.68	113.12
1	F	43	LEU	N-CA-C	-6.75	104.69	113.12
1	B	43	LEU	N-CA-C	-6.74	104.69	113.12
1	F	129	TRP	CB-CA-C	-6.70	99.22	110.81
1	A	89	LEU	N-CA-C	-6.70	104.13	112.90
1	E	89	LEU	N-CA-C	-6.70	104.13	112.90
1	B	129	TRP	CB-CA-C	-6.69	99.24	110.81
1	B	395	ARG	N-CA-CB	-6.66	100.94	110.79
1	C	227	THR	N-CA-C	6.62	121.56	112.04
1	E	138	LEU	N-CA-C	6.60	120.36	110.14
1	C	149	ARG	N-CA-C	-6.59	99.43	109.85
1	A	399	GLN	N-CA-C	6.59	119.33	109.25
1	H	53	ASP	N-CA-C	6.58	120.92	113.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	53	ASP	N-CA-C	6.58	120.91	113.02
1	H	442	ARG	CA-C-N	-6.57	109.52	120.30
1	H	442	ARG	C-N-CA	-6.57	109.52	120.30
1	B	53	ASP	N-CA-C	6.57	120.90	113.02
1	F	53	ASP	N-CA-C	6.57	120.90	113.02
1	C	53	ASP	N-CA-C	6.56	120.89	113.02
1	E	53	ASP	N-CA-C	6.55	120.88	113.02
1	A	53	ASP	N-CA-C	6.54	120.87	113.02
1	F	391	LYS	N-CA-C	6.53	120.19	111.30
1	G	53	ASP	N-CA-C	6.53	120.86	113.02
1	E	123	LEU	CB-CA-C	6.51	120.99	110.96
1	A	123	LEU	CB-CA-C	6.50	120.97	110.96
1	D	123	LEU	CB-CA-C	6.50	121.03	110.95
1	B	123	LEU	CB-CA-C	6.50	120.97	110.96
1	H	123	LEU	CB-CA-C	6.50	121.02	110.95
1	F	123	LEU	CB-CA-C	6.49	120.96	110.96
1	H	281	ASP	CA-C-N	6.47	126.23	119.05
1	H	281	ASP	C-N-CA	6.47	126.23	119.05
1	D	281	ASP	CA-C-N	6.47	126.23	119.05
1	D	281	ASP	C-N-CA	6.47	126.23	119.05
1	C	123	LEU	CB-CA-C	6.46	120.96	110.95
1	E	281	ASP	CA-C-N	6.44	126.20	119.05
1	E	281	ASP	C-N-CA	6.44	126.20	119.05
1	H	67	SER	O-C-N	-6.44	115.90	123.11
1	B	148	VAL	N-CA-C	-6.43	95.96	109.34
1	G	123	LEU	CB-CA-C	6.43	120.92	110.95
1	C	281	ASP	CA-C-N	6.43	126.18	119.05
1	C	281	ASP	C-N-CA	6.43	126.18	119.05
1	A	281	ASP	CA-C-N	6.42	126.17	119.05
1	A	281	ASP	C-N-CA	6.42	126.17	119.05
1	D	67	SER	O-C-N	-6.41	115.93	123.11
1	G	415	ALA	N-CA-C	6.40	120.19	112.38
1	C	415	ALA	N-CA-C	6.39	120.17	112.38
1	B	138	LEU	N-CA-C	6.36	119.38	109.52
1	F	138	LEU	N-CA-C	6.36	119.38	109.52
1	D	138	LEU	N-CA-C	6.35	119.37	109.52
1	F	51	VAL	CA-C-N	6.33	129.05	120.44
1	F	51	VAL	C-N-CA	6.33	129.05	120.44
1	E	422	ASN	CB-CA-C	-6.30	101.29	111.06
1	E	51	VAL	CA-C-N	6.30	129.01	120.44
1	E	51	VAL	C-N-CA	6.30	129.01	120.44
1	B	390	GLU	N-CA-CB	-6.30	106.99	114.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	VAL	CA-C-N	6.30	129.00	120.44
1	B	51	VAL	C-N-CA	6.30	129.00	120.44
1	A	422	ASN	CB-CA-C	-6.29	101.31	111.06
1	B	422	ASN	CB-CA-C	-6.27	101.34	111.06
1	C	422	ASN	CB-CA-C	-6.27	101.34	111.06
1	G	51	VAL	CA-C-N	6.27	128.97	120.44
1	G	51	VAL	C-N-CA	6.27	128.97	120.44
1	D	422	ASN	CB-CA-C	-6.27	101.34	111.06
1	C	51	VAL	CA-C-N	6.27	128.96	120.44
1	C	51	VAL	C-N-CA	6.27	128.96	120.44
1	A	51	VAL	CA-C-N	6.26	128.95	120.44
1	A	51	VAL	C-N-CA	6.26	128.95	120.44
1	E	197	THR	CB-CA-C	-6.26	102.17	110.87
1	G	197	THR	CB-CA-C	-6.25	102.18	110.87
1	H	422	ASN	CB-CA-C	-6.25	101.37	111.06
1	D	51	VAL	CA-C-N	6.25	128.94	120.44
1	D	51	VAL	C-N-CA	6.25	128.94	120.44
1	H	51	VAL	CA-C-N	6.25	128.94	120.44
1	H	51	VAL	C-N-CA	6.25	128.94	120.44
1	A	371	THR	CA-C-N	6.25	129.74	120.87
1	A	371	THR	C-N-CA	6.25	129.74	120.87
1	C	197	THR	CB-CA-C	-6.25	102.19	110.87
1	C	138	LEU	N-CA-C	6.25	119.37	109.50
1	F	53	ASP	CB-CA-C	-6.25	99.25	110.37
1	F	422	ASN	CB-CA-C	-6.24	101.38	111.06
1	G	422	ASN	CB-CA-C	-6.24	101.39	111.06
1	F	197	THR	CB-CA-C	-6.23	102.21	110.87
1	B	53	ASP	CB-CA-C	-6.23	99.28	110.37
1	D	147	GLU	N-CA-CB	-6.23	107.07	114.17
1	G	138	LEU	N-CA-C	6.23	119.34	109.50
1	A	53	ASP	CB-CA-C	-6.22	99.29	110.37
1	D	53	ASP	CB-CA-C	-6.22	99.30	110.37
1	G	53	ASP	CB-CA-C	-6.22	99.29	110.37
1	C	53	ASP	CB-CA-C	-6.21	99.31	110.37
1	E	53	ASP	CB-CA-C	-6.21	99.31	110.37
1	H	197	THR	CB-CA-C	-6.20	102.26	110.87
1	H	53	ASP	CB-CA-C	-6.19	99.36	110.37
1	H	147	GLU	N-CA-CB	-6.19	107.12	114.17
1	A	394	ILE	N-CA-C	-6.14	96.58	109.34
1	C	371	THR	CB-CA-C	-6.13	99.32	109.99
1	B	394	ILE	CB-CA-C	-6.11	101.26	111.29
1	G	293	ILE	CB-CA-C	-6.11	101.27	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	427	GLY	CA-C-N	6.10	128.38	120.44
1	D	427	GLY	C-N-CA	6.10	128.38	120.44
1	G	148	VAL	CB-CA-C	6.09	119.23	110.33
1	C	293	ILE	CB-CA-C	-6.09	101.30	111.29
1	F	293	ILE	CB-CA-C	-6.09	101.30	111.29
1	A	436	ASP	CB-CA-C	-6.09	100.95	111.30
1	E	61	ALA	N-CA-C	-6.08	105.68	113.23
1	B	123	LEU	N-CA-C	-6.08	104.34	110.97
1	D	61	ALA	N-CA-C	-6.08	105.69	113.23
1	B	293	ILE	CB-CA-C	-6.08	101.32	111.29
1	E	436	ASP	CB-CA-C	-6.08	100.97	111.30
1	D	88	LEU	CB-CA-C	-6.08	100.29	110.56
1	H	61	ALA	N-CA-C	-6.08	105.69	113.23
1	A	293	ILE	CB-CA-C	-6.07	101.33	111.29
1	E	123	LEU	N-CA-C	-6.07	104.35	110.97
1	B	61	ALA	N-CA-C	-6.07	105.70	113.23
1	F	61	ALA	N-CA-C	-6.07	105.70	113.23
1	F	436	ASP	CB-CA-C	-6.07	100.98	111.30
1	A	123	LEU	N-CA-C	-6.07	104.36	110.97
1	F	123	LEU	N-CA-C	-6.07	104.36	110.97
1	B	40	GLY	N-CA-C	-6.06	98.81	113.18
1	H	88	LEU	CB-CA-C	-6.06	100.31	110.56
1	A	61	ALA	N-CA-C	-6.06	105.71	113.23
1	H	123	LEU	N-CA-C	-6.06	104.30	111.03
1	E	293	ILE	CB-CA-C	-6.06	101.35	111.29
1	H	293	ILE	CB-CA-C	-6.06	101.35	111.29
1	D	293	ILE	CB-CA-C	-6.06	101.35	111.29
1	G	61	ALA	N-CA-C	-6.06	105.72	113.23
1	A	394	ILE	CB-CA-C	-6.06	101.36	111.29
1	C	61	ALA	N-CA-C	-6.03	105.75	113.23
1	F	226	GLU	N-CA-C	-6.03	105.02	112.38
1	D	123	LEU	N-CA-C	-6.03	104.34	111.03
1	A	138	LEU	N-CA-C	6.02	118.85	109.52
1	C	389	ARG	N-CA-C	-6.02	102.16	110.35
1	C	123	LEU	N-CA-C	-6.01	104.35	111.03
1	G	123	LEU	N-CA-C	-6.01	104.36	111.03
1	G	414	ILE	N-CA-C	6.01	118.56	111.05
1	C	89	LEU	N-CA-C	-6.00	104.11	112.45
1	G	89	LEU	N-CA-C	-6.00	104.11	112.45
1	E	392	LYS	N-CA-C	-5.99	100.43	109.95
1	E	428	LEU	N-CA-CB	-5.99	101.17	109.91
1	B	436	ASP	CB-CA-C	-5.98	100.95	111.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	98	ARG	CB-CA-C	5.96	120.67	110.79
1	C	98	ARG	CB-CA-C	5.94	120.64	110.79
1	G	428	LEU	N-CA-C	5.94	118.64	111.40
1	B	142	LEU	N-CA-C	5.93	122.91	109.81
1	A	98	ARG	CB-CA-C	5.91	120.61	110.79
1	E	470	LYS	N-CA-C	5.91	118.54	108.67
1	D	98	ARG	CB-CA-C	5.91	120.59	110.79
1	G	395	ARG	CB-CA-C	-5.91	99.43	110.36
1	B	98	ARG	CB-CA-C	5.90	120.58	110.79
1	F	470	LYS	N-CA-C	5.90	118.52	108.67
1	A	470	LYS	N-CA-C	5.89	118.51	108.67
1	F	88	LEU	CB-CA-C	-5.89	100.25	110.09
1	B	88	LEU	CB-CA-C	-5.89	100.25	110.09
1	E	88	LEU	CB-CA-C	-5.89	100.25	110.09
1	H	98	ARG	CB-CA-C	5.89	120.57	110.79
1	F	394	ILE	N-CA-C	5.89	120.28	112.04
1	D	470	LYS	N-CA-C	5.88	118.50	108.67
1	E	98	ARG	CB-CA-C	5.88	120.56	110.79
1	F	98	ARG	CB-CA-C	5.88	120.56	110.79
1	B	470	LYS	N-CA-C	5.88	118.49	108.67
1	A	88	LEU	CB-CA-C	-5.88	100.27	110.09
1	C	470	LYS	N-CA-C	5.88	118.49	108.67
1	G	470	LYS	N-CA-C	5.88	118.48	108.67
1	H	39	THR	N-CA-C	-5.87	106.03	113.43
1	G	88	LEU	CB-CA-C	-5.86	100.30	110.09
1	C	88	LEU	CB-CA-C	-5.86	100.31	110.09
1	H	470	LYS	N-CA-C	5.85	118.44	108.67
1	A	176	VAL	N-CA-C	-5.83	104.82	110.42
1	G	390	GLU	N-CA-CB	-5.83	107.52	114.17
1	E	176	VAL	N-CA-C	-5.82	104.84	110.42
1	C	452	VAL	N-CA-C	5.79	117.09	109.21
1	H	82	LEU	CA-C-N	5.79	128.51	120.29
1	H	82	LEU	C-N-CA	5.79	128.51	120.29
1	B	452	VAL	N-CA-C	5.78	117.08	109.21
1	C	422	ASN	N-CA-C	5.78	119.10	112.57
1	F	452	VAL	N-CA-C	5.78	117.07	109.21
1	H	452	VAL	N-CA-C	5.78	117.07	109.21
1	H	422	ASN	N-CA-C	5.78	119.10	112.57
1	A	422	ASN	N-CA-C	5.78	119.10	112.57
1	F	422	ASN	N-CA-C	5.78	119.10	112.57
1	B	422	ASN	N-CA-C	5.77	119.09	112.57
1	D	452	VAL	N-CA-C	5.77	117.06	109.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	422	ASN	N-CA-C	5.77	119.09	112.57
1	D	148	VAL	CB-CA-C	5.77	119.17	110.63
1	E	452	VAL	N-CA-C	5.77	117.06	109.21
1	A	452	VAL	N-CA-C	5.77	117.05	109.21
1	G	452	VAL	N-CA-C	5.77	117.05	109.21
1	D	36	ASN	N-CA-C	-5.76	101.26	109.62
1	D	82	LEU	CA-C-N	5.76	128.47	120.29
1	D	82	LEU	C-N-CA	5.76	128.47	120.29
1	H	148	VAL	CB-CA-C	5.75	119.14	110.63
1	B	412	SER	N-CA-C	5.75	120.32	112.04
1	G	422	ASN	N-CA-C	5.75	119.07	112.57
1	B	64	THR	CB-CA-C	-5.75	97.88	109.55
1	F	64	THR	CB-CA-C	-5.75	97.88	109.55
1	D	422	ASN	N-CA-C	5.74	119.05	112.57
1	E	82	LEU	CA-C-N	5.74	128.44	120.29
1	E	82	LEU	C-N-CA	5.74	128.44	120.29
1	E	197	THR	N-CA-C	5.74	118.29	108.82
1	F	412	SER	N-CA-C	5.73	120.30	112.04
1	A	82	LEU	CA-C-N	5.73	128.43	120.29
1	A	82	LEU	C-N-CA	5.73	128.43	120.29
1	C	197	THR	N-CA-C	5.73	118.27	108.82
1	A	412	SER	N-CA-C	5.72	120.28	112.04
1	C	412	SER	N-CA-C	5.72	120.28	112.04
1	G	197	THR	N-CA-C	5.72	118.26	108.82
1	B	146	PRO	N-CA-C	-5.72	100.69	112.47
1	E	412	SER	N-CA-C	5.71	120.27	112.04
1	H	138	LEU	N-CA-C	5.70	117.90	109.69
1	H	142	LEU	N-CA-C	5.70	122.40	109.81
1	H	197	THR	N-CA-C	5.70	118.22	108.82
1	F	197	THR	N-CA-C	5.70	118.22	108.82
1	G	412	SER	N-CA-C	5.70	120.24	112.04
1	E	139	ASP	O-C-N	-5.69	116.69	123.06
1	D	412	SER	N-CA-C	5.68	120.25	111.56
1	H	412	SER	N-CA-C	5.68	120.25	111.56
1	G	359	GLY	N-CA-C	5.67	120.66	113.24
1	C	359	GLY	N-CA-C	5.66	120.66	113.24
1	E	378	GLY	N-CA-C	5.66	117.81	112.04
1	G	378	GLY	N-CA-C	5.65	117.81	112.04
1	C	417	VAL	N-CA-C	-5.63	104.41	112.35
1	A	378	GLY	N-CA-C	5.63	117.78	112.04
1	B	378	GLY	N-CA-C	5.63	117.78	112.04
1	C	378	GLY	N-CA-C	5.62	117.78	112.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	378	GLY	N-CA-C	5.61	117.76	112.04
1	H	378	GLY	N-CA-C	5.60	117.75	112.04
1	A	443	ILE	N-CA-C	-5.60	105.27	110.53
1	F	300	VAL	N-CA-CB	5.60	120.47	111.23
1	G	417	VAL	N-CA-C	-5.60	104.46	112.35
1	H	300	VAL	N-CA-CB	5.60	120.46	111.23
1	B	300	VAL	N-CA-CB	5.59	120.46	111.23
1	B	37	PRO	N-CA-C	-5.59	106.82	114.98
1	B	443	ILE	N-CA-C	-5.59	105.28	110.53
1	A	300	VAL	N-CA-CB	5.58	120.44	111.23
1	D	300	VAL	N-CA-CB	5.58	120.44	111.23
1	C	300	VAL	N-CA-CB	5.58	120.44	111.23
1	G	320	ARG	N-CA-C	-5.58	105.11	111.14
1	F	378	GLY	N-CA-C	5.58	117.73	112.04
1	E	443	ILE	N-CA-C	-5.58	105.29	110.53
1	G	300	VAL	N-CA-CB	5.58	120.43	111.23
1	A	129	TRP	N-CA-C	-5.57	105.60	112.90
1	C	320	ARG	N-CA-C	-5.57	105.12	111.14
1	E	300	VAL	N-CA-CB	5.57	120.42	111.23
1	E	129	TRP	N-CA-C	-5.57	105.61	112.90
1	F	226	GLU	CA-C-N	-5.56	110.91	121.54
1	F	226	GLU	C-N-CA	-5.56	110.91	121.54
1	A	320	ARG	N-CA-C	-5.56	105.14	111.14
1	A	142	LEU	N-CA-C	5.55	122.09	109.81
1	H	323	VAL	N-CA-C	-5.55	105.11	110.72
1	E	320	ARG	N-CA-C	-5.55	105.14	111.14
1	D	320	ARG	N-CA-C	-5.55	105.15	111.14
1	F	323	VAL	N-CA-C	-5.55	105.12	110.72
1	D	356	ILE	N-CA-C	-5.54	105.10	110.42
1	F	443	ILE	N-CA-C	-5.54	105.32	110.53
1	H	320	ARG	N-CA-C	-5.54	105.16	111.14
1	B	323	VAL	N-CA-C	-5.54	105.13	110.72
1	G	356	ILE	N-CA-C	-5.53	105.11	110.42
1	F	356	ILE	N-CA-C	-5.53	105.11	110.42
1	H	356	ILE	N-CA-C	-5.53	105.11	110.42
1	B	320	ARG	N-CA-C	-5.53	105.17	111.14
1	D	323	VAL	N-CA-C	-5.53	105.14	110.72
1	A	323	VAL	N-CA-C	-5.53	105.14	110.72
1	G	137	THR	N-CA-C	-5.53	99.28	108.34
1	C	356	ILE	N-CA-C	-5.53	105.11	110.42
1	E	356	ILE	N-CA-C	-5.52	105.12	110.42
1	F	320	ARG	N-CA-C	-5.52	105.17	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	323	VAL	N-CA-C	-5.52	105.14	110.72
1	D	137	THR	N-CA-C	-5.52	99.29	108.34
1	F	59	GLU	N-CA-C	-5.52	106.71	113.50
1	G	323	VAL	N-CA-C	-5.52	105.15	110.72
1	C	137	THR	N-CA-C	-5.52	99.29	108.34
1	A	356	ILE	N-CA-C	-5.51	105.13	110.42
1	A	436	ASP	N-CA-C	5.51	117.69	107.99
1	H	59	GLU	N-CA-C	-5.51	106.72	113.50
1	C	323	VAL	N-CA-C	-5.51	105.16	110.72
1	H	137	THR	N-CA-C	-5.51	99.31	108.34
1	B	356	ILE	N-CA-C	-5.50	105.14	110.42
1	A	137	THR	N-CA-C	-5.50	99.31	108.34
1	F	436	ASP	N-CA-C	5.50	117.67	107.99
1	D	59	GLU	N-CA-C	-5.50	106.74	113.50
1	B	436	ASP	N-CA-C	5.50	117.69	108.23
1	G	327	SER	N-CA-C	5.50	119.69	113.15
1	C	327	SER	N-CA-C	5.50	119.69	113.15
1	B	59	GLU	N-CA-C	-5.49	106.74	113.50
1	E	436	ASP	N-CA-C	5.49	117.65	107.99
1	F	327	SER	N-CA-C	5.49	119.68	113.15
1	G	59	GLU	N-CA-C	-5.49	106.75	113.50
1	G	391	LYS	N-CA-CB	-5.48	102.98	111.65
1	A	428	LEU	N-CA-CB	-5.48	102.03	110.20
1	A	59	GLU	N-CA-C	-5.48	106.76	113.50
1	E	59	GLU	N-CA-C	-5.48	106.76	113.50
1	E	411	PHE	N-CA-C	5.48	117.42	108.55
1	A	371	THR	CB-CA-C	-5.48	100.46	109.99
1	B	137	THR	N-CA-C	-5.48	99.36	108.34
1	C	59	GLU	N-CA-C	-5.48	106.76	113.50
1	G	389	ARG	CB-CA-C	5.48	119.42	109.62
1	E	327	SER	N-CA-C	5.47	119.67	113.15
1	F	137	THR	N-CA-C	-5.47	99.36	108.34
1	D	72	ARG	CA-C-N	5.46	127.99	120.67
1	D	72	ARG	C-N-CA	5.46	127.99	120.67
1	E	441	LEU	N-CA-C	5.46	118.16	111.82
1	A	327	SER	N-CA-C	5.46	119.65	113.15
1	B	63	ALA	O-C-N	5.46	128.38	122.15
1	B	327	SER	N-CA-C	5.46	119.65	113.15
1	D	327	SER	N-CA-C	5.46	119.64	113.15
1	E	56	ALA	N-CA-C	-5.45	105.25	111.14
1	A	411	PHE	N-CA-C	5.45	117.38	108.55
1	G	426	TYR	CB-CA-C	-5.45	100.66	110.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	411	PHE	N-CA-C	5.45	117.38	108.55
1	H	327	SER	N-CA-C	5.45	119.63	113.15
1	B	131	THR	N-CA-CB	-5.44	101.92	110.46
1	H	72	ARG	CA-C-N	5.44	127.96	120.67
1	H	72	ARG	C-N-CA	5.44	127.96	120.67
1	F	131	THR	N-CA-CB	-5.44	101.92	110.46
1	G	393	ASP	N-CA-C	-5.44	99.93	108.63
1	H	324	ILE	N-CA-C	5.44	116.17	110.62
1	C	324	ILE	N-CA-C	5.44	116.17	110.62
1	D	324	ILE	N-CA-C	5.43	116.16	110.62
1	A	324	ILE	N-CA-C	5.43	116.16	110.62
1	A	441	LEU	N-CA-C	5.43	118.12	111.82
1	G	411	PHE	N-CA-C	5.43	117.35	108.55
1	B	141	SER	N-CA-C	-5.43	95.77	107.49
1	B	411	PHE	N-CA-C	5.43	117.34	108.55
1	D	411	PHE	N-CA-C	5.43	117.34	108.55
1	F	63	ALA	O-C-N	5.43	128.34	122.15
1	H	411	PHE	N-CA-C	5.43	117.34	108.55
1	B	56	ALA	N-CA-C	-5.42	105.28	111.14
1	B	324	ILE	N-CA-C	5.42	116.15	110.62
1	F	199	LEU	N-CA-C	5.42	117.19	111.28
1	A	56	ALA	N-CA-C	-5.42	105.29	111.14
1	F	441	LEU	N-CA-C	5.42	118.11	111.82
1	G	324	ILE	N-CA-C	5.42	116.15	110.62
1	F	411	PHE	N-CA-C	5.42	117.32	108.55
1	B	197	THR	N-CA-C	5.41	118.24	108.55
1	D	56	ALA	N-CA-C	-5.41	105.30	111.14
1	H	175	ALA	N-CA-C	5.41	116.86	111.07
1	H	56	ALA	N-CA-C	-5.41	105.30	111.14
1	A	72	ARG	CA-C-N	5.41	127.92	120.67
1	A	72	ARG	C-N-CA	5.41	127.92	120.67
1	A	197	THR	N-CA-C	5.41	118.23	108.55
1	B	441	LEU	N-CA-C	5.41	118.09	111.82
1	D	197	THR	N-CA-C	5.41	118.22	108.55
1	E	324	ILE	N-CA-C	5.40	116.13	110.62
1	B	72	ARG	CA-C-N	5.40	127.91	120.67
1	B	72	ARG	C-N-CA	5.40	127.91	120.67
1	F	56	ALA	N-CA-C	-5.40	105.31	111.14
1	E	72	ARG	CA-C-N	5.40	127.90	120.67
1	E	72	ARG	C-N-CA	5.40	127.90	120.67
1	E	199	LEU	N-CA-C	5.40	117.16	111.28
1	B	199	LEU	N-CA-C	5.40	117.16	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	ALA	N-CA-C	5.39	116.84	111.07
1	D	175	ALA	N-CA-C	5.39	116.84	111.07
1	C	175	ALA	N-CA-C	5.39	116.83	111.07
1	A	16	GLN	N-CA-C	-5.38	95.93	111.00
1	C	199	LEU	N-CA-C	5.38	117.15	111.28
1	F	72	ARG	CA-C-N	5.38	127.88	120.67
1	F	72	ARG	C-N-CA	5.38	127.88	120.67
1	F	324	ILE	N-CA-C	5.38	116.11	110.62
1	G	175	ALA	N-CA-C	5.38	116.83	111.07
1	A	199	LEU	N-CA-C	5.38	117.14	111.28
1	A	477	GLU	N-CA-C	5.38	119.84	113.12
1	D	199	LEU	N-CA-C	5.38	117.14	111.28
1	C	72	ARG	CA-C-N	5.37	127.87	120.67
1	C	72	ARG	C-N-CA	5.37	127.87	120.67
1	G	199	LEU	N-CA-C	5.37	117.14	111.28
1	E	16	GLN	N-CA-C	-5.37	95.97	111.00
1	C	56	ALA	N-CA-C	-5.37	105.34	111.14
1	F	175	ALA	N-CA-C	5.37	116.81	111.07
1	E	477	GLU	N-CA-C	5.36	119.81	113.12
1	G	56	ALA	N-CA-C	-5.36	105.36	111.14
1	C	443	ILE	N-CA-C	-5.35	105.28	110.42
1	H	199	LEU	N-CA-C	5.35	117.11	111.28
1	G	443	ILE	N-CA-C	-5.34	105.29	110.42
1	D	293	ILE	N-CA-C	5.33	120.43	109.34
1	F	293	ILE	N-CA-C	5.33	120.43	109.34
1	G	293	ILE	N-CA-C	5.33	120.43	109.34
1	G	72	ARG	CA-C-N	5.33	127.81	120.67
1	G	72	ARG	C-N-CA	5.33	127.81	120.67
1	B	293	ILE	N-CA-C	5.33	120.42	109.34
1	A	293	ILE	N-CA-C	5.32	120.41	109.34
1	C	293	ILE	N-CA-C	5.32	120.41	109.34
1	H	293	ILE	N-CA-C	5.31	120.39	109.34
1	E	293	ILE	N-CA-C	5.30	120.37	109.34
1	F	176	VAL	N-CA-C	-5.30	104.80	110.36
1	A	397	LEU	N-CA-C	-5.27	106.80	113.18
1	D	441	LEU	CA-C-N	5.27	127.87	120.28
1	D	441	LEU	C-N-CA	5.27	127.87	120.28
1	B	176	VAL	N-CA-C	-5.26	104.83	110.36
1	E	438	SER	CB-CA-C	5.26	119.07	110.96
1	A	438	SER	CB-CA-C	5.26	119.06	110.96
1	F	438	SER	CB-CA-C	5.26	119.05	110.96
1	D	442	ARG	CA-C-N	-5.25	111.69	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	442	ARG	C-N-CA	-5.25	111.69	120.30
1	B	438	SER	CB-CA-C	5.25	119.04	110.96
1	H	176	VAL	CB-CA-C	5.25	118.42	111.70
1	H	438	SER	CB-CA-C	5.24	119.04	110.96
1	B	16	GLN	N-CA-C	-5.24	96.33	111.00
1	D	438	SER	CB-CA-C	5.24	119.03	110.96
1	F	236	PRO	CB-CA-C	-5.24	104.04	112.21
1	E	426	TYR	CB-CA-C	5.22	119.11	109.71
1	A	236	PRO	CB-CA-C	-5.22	104.07	112.21
1	E	110	TYR	N-CA-C	5.22	118.91	112.54
1	E	236	PRO	CB-CA-C	-5.22	104.07	112.21
1	B	236	PRO	CB-CA-C	-5.22	104.07	112.21
1	D	176	VAL	CB-CA-C	5.22	118.38	111.70
1	D	236	PRO	CB-CA-C	-5.20	104.09	112.21
1	D	142	LEU	N-CA-C	5.20	121.31	109.81
1	D	110	TYR	N-CA-C	5.20	118.88	112.54
1	D	176	VAL	N-CA-C	-5.20	104.83	110.23
1	G	389	ARG	N-CA-C	-5.19	103.29	110.35
1	G	236	PRO	CB-CA-C	-5.19	104.11	112.21
1	F	177	TRP	N-CA-C	5.19	119.09	112.34
1	H	110	TYR	N-CA-C	5.19	118.87	112.54
1	C	236	PRO	CB-CA-C	-5.18	104.12	112.21
1	D	413	ASP	CB-CA-C	-5.18	100.38	109.71
1	A	110	TYR	N-CA-C	5.18	118.86	112.54
1	H	236	PRO	CB-CA-C	-5.18	104.12	112.21
1	E	174	MET	CA-C-N	5.18	127.65	120.29
1	E	174	MET	C-N-CA	5.18	127.65	120.29
1	B	177	TRP	N-CA-C	5.18	119.07	112.34
1	A	174	MET	CA-C-N	5.17	127.64	120.29
1	A	174	MET	C-N-CA	5.17	127.64	120.29
1	H	176	VAL	N-CA-C	-5.17	104.85	110.23
1	H	413	ASP	CB-CA-C	-5.17	100.40	109.71
1	F	110	TYR	N-CA-C	5.16	118.83	112.54
1	B	110	TYR	N-CA-C	5.16	118.83	112.54
1	F	63	ALA	CA-C-N	5.16	130.73	121.66
1	F	63	ALA	C-N-CA	5.16	130.73	121.66
1	G	221	VAL	O-C-N	-5.16	117.46	122.93
1	E	221	VAL	O-C-N	-5.14	117.48	122.93
1	C	221	VAL	O-C-N	-5.14	117.48	122.93
1	B	221	VAL	O-C-N	-5.13	117.49	122.93
1	A	221	VAL	O-C-N	-5.13	117.49	122.93
1	B	63	ALA	CA-C-N	5.13	130.68	121.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	ALA	C-N-CA	5.13	130.68	121.66
1	D	221	VAL	O-C-N	-5.12	117.50	122.93
1	A	370	GLY	CA-C-O	-5.12	117.38	120.91
1	F	270	GLY	O-C-N	-5.11	118.81	123.36
1	B	176	VAL	CB-CA-C	5.10	118.41	111.88
1	C	235	HIS	CB-CA-C	5.09	116.67	109.08
1	G	143	PRO	CA-N-CD	-5.09	104.38	111.50
1	H	221	VAL	O-C-N	-5.09	117.54	122.93
1	A	235	HIS	CB-CA-C	5.08	116.65	109.08
1	G	235	HIS	CB-CA-C	5.08	116.65	109.08
1	F	176	VAL	CB-CA-C	5.08	118.38	111.88
1	D	235	HIS	CB-CA-C	5.08	116.64	109.08
1	F	221	VAL	O-C-N	-5.08	117.55	122.93
1	G	76	SER	N-CA-C	-5.08	106.50	113.30
1	E	143	PRO	N-CA-CB	5.07	108.18	102.60
1	F	76	SER	N-CA-C	-5.07	106.50	113.30
1	B	76	SER	N-CA-C	-5.07	106.51	113.30
1	A	76	SER	N-CA-C	-5.06	106.52	113.30
1	B	235	HIS	CB-CA-C	5.06	116.62	109.08
1	E	235	HIS	CB-CA-C	5.06	116.61	109.08
1	F	235	HIS	CB-CA-C	5.06	116.62	109.08
1	G	418	VAL	N-CA-C	-5.06	105.61	110.72
1	C	76	SER	N-CA-C	-5.05	106.53	113.30
1	H	235	HIS	CB-CA-C	5.05	116.61	109.08
1	E	76	SER	N-CA-C	-5.05	106.53	113.30
1	H	390	GLU	N-CA-CB	-5.05	105.99	114.27
1	H	76	SER	N-CA-C	-5.04	106.55	113.30
1	C	418	VAL	N-CA-C	-5.04	105.63	110.72
1	D	76	SER	N-CA-C	-5.02	106.57	113.30
1	D	390	GLU	N-CA-CB	-5.02	106.04	114.27
1	G	128	GLY	N-CA-C	5.00	121.51	115.31
1	A	418	VAL	N-CA-C	-5.00	105.67	110.72

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	141	SER	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	0	3298	164	0
1	B	3411	0	3298	135	0
1	C	3409	0	3292	142	0
1	D	3419	0	3314	134	0
1	E	3408	0	3290	152	0
1	F	3411	0	3298	125	0
1	G	3419	0	3309	120	0
1	H	3413	0	3303	141	0
All	All	27306	0	26402	1050	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1050) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ARG:CG	1:C:487:THR:HG21	1.58	1.34
1:B:397:LEU:CD1	1:B:407:VAL:HG11	1.57	1.34
1:E:156:ARG:CG	1:E:487:THR:HG21	1.58	1.33
1:B:156:ARG:CG	1:B:487:THR:HG21	1.58	1.33
1:G:156:ARG:CG	1:G:487:THR:HG21	1.58	1.32
1:A:156:ARG:CG	1:A:487:THR:HG21	1.58	1.30
1:A:241:VAL:HG11	1:A:257:CYS:SG	1.73	1.28
1:G:139:ASP:O	1:G:140:LEU:HD23	1.28	1.28
1:C:156:ARG:HG3	1:C:487:THR:CG2	1.76	1.16
1:A:156:ARG:HG3	1:A:487:THR:CG2	1.76	1.16
1:B:142:LEU:HB2	1:B:143:PRO:CA	1.77	1.15
1:H:271:LYS:HE3	1:H:306:ARG:CG	1.75	1.15
1:G:156:ARG:HG3	1:G:487:THR:CG2	1.76	1.14
1:B:142:LEU:CB	1:B:143:PRO:HA	1.69	1.14
1:E:156:ARG:HG3	1:E:487:THR:CG2	1.76	1.14
1:B:156:ARG:HG3	1:B:487:THR:CG2	1.76	1.14
1:D:139:ASP:O	1:D:140:LEU:CD1	1.96	1.13
1:A:79:GLU:O	1:A:83:LEU:HD13	1.48	1.13
1:H:142:LEU:HB2	1:H:143:PRO:HA	1.13	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LEU:CD1	1:A:407:VAL:HG11	1.80	1.12
1:E:79:GLU:O	1:E:83:LEU:HD13	1.48	1.11
1:A:142:LEU:HB2	1:A:143:PRO:HA	1.34	1.10
1:A:114:MET:HE1	1:A:295:PHE:CE1	1.87	1.10
1:A:394:ILE:HD13	1:A:394:ILE:N	1.52	1.10
1:D:139:ASP:O	1:D:140:LEU:HD12	1.53	1.08
1:F:139:ASP:O	1:F:140:LEU:HG	1.52	1.08
1:A:397:LEU:HD12	1:A:407:VAL:HG11	1.33	1.07
1:F:140:LEU:HD11	1:F:152:ALA:HB2	1.16	1.07
1:B:397:LEU:HD12	1:B:407:VAL:HG11	1.16	1.07
1:D:142:LEU:HB2	1:D:143:PRO:HA	1.11	1.07
1:H:396:LEU:HD23	1:H:407:VAL:HB	1.33	1.06
1:C:142:LEU:CB	1:C:143:PRO:HA	1.84	1.06
1:H:271:LYS:HE3	1:H:306:ARG:HG3	1.09	1.06
1:B:283:GLN:OE1	1:B:320:ARG:HD3	1.54	1.04
1:B:139:ASP:O	1:B:140:LEU:HD13	1.57	1.04
1:F:283:GLN:HG2	1:F:320:ARG:HD3	1.39	1.03
1:A:362:ASP:HB3	1:A:394:ILE:HG23	1.41	1.02
1:A:394:ILE:HD13	1:A:394:ILE:H	0.88	1.02
1:A:156:ARG:HG3	1:A:487:THR:HG21	1.02	1.01
1:A:241:VAL:CG1	1:A:257:CYS:SG	2.48	1.01
1:C:156:ARG:HG3	1:C:487:THR:HG21	1.02	1.01
1:E:156:ARG:HG3	1:E:487:THR:HG21	1.02	1.01
1:C:142:LEU:HB2	1:C:143:PRO:HA	1.02	1.00
1:E:139:ASP:O	1:E:140:LEU:HD23	1.60	0.99
1:H:142:LEU:HB2	1:H:143:PRO:CA	1.91	0.99
1:G:156:ARG:HG3	1:G:487:THR:HG21	1.02	0.99
1:E:144:LEU:HB3	1:E:145:PRO:HD2	1.45	0.99
1:A:139:ASP:HB2	1:D:75:PRO:HG2	1.45	0.99
1:F:140:LEU:HD11	1:F:152:ALA:CB	1.92	0.99
1:F:142:LEU:HB2	1:F:143:PRO:HA	1.46	0.98
1:C:144:LEU:HB3	1:C:148:VAL:HG11	1.45	0.98
1:E:139:ASP:HB2	1:H:75:PRO:HG2	1.46	0.98
1:B:156:ARG:HG3	1:B:487:THR:HG21	1.02	0.97
1:C:142:LEU:HB2	1:C:143:PRO:CA	1.94	0.97
1:B:397:LEU:CD1	1:B:407:VAL:CG1	2.42	0.97
1:H:425:VAL:O	1:H:471:ASP:HB2	1.66	0.96
1:C:413:ASP:OD1	1:C:416:GLU:HG2	1.65	0.95
1:B:139:ASP:HB2	1:C:75:PRO:HG2	1.48	0.95
1:D:142:LEU:HB2	1:D:143:PRO:CA	1.98	0.94
1:E:118:ALA:O	1:E:122:TRP:HD1	1.50	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ASP:O	1:B:140:LEU:CD1	2.17	0.92
1:A:118:ALA:O	1:A:122:TRP:HD1	1.50	0.92
1:E:122:TRP:HZ3	1:E:478:HIS:ND1	1.67	0.92
1:F:139:ASP:O	1:F:140:LEU:CG	2.18	0.92
1:E:397:LEU:HD12	1:E:407:VAL:HG11	1.50	0.92
1:E:144:LEU:HB3	1:E:145:PRO:CD	1.98	0.90
1:A:139:ASP:O	1:A:140:LEU:HD12	1.71	0.90
1:A:122:TRP:HZ3	1:A:478:HIS:ND1	1.67	0.89
1:D:142:LEU:CB	1:D:143:PRO:HA	1.93	0.89
1:H:396:LEU:CD2	1:H:407:VAL:HB	2.02	0.89
1:A:114:MET:HE1	1:A:295:PHE:HE1	1.32	0.89
1:C:144:LEU:HD13	1:C:148:VAL:CG1	2.00	0.89
1:A:394:ILE:H	1:A:394:ILE:CD1	1.73	0.88
1:D:139:ASP:O	1:D:140:LEU:HD13	1.71	0.88
1:E:140:LEU:HD11	1:E:152:ALA:CB	2.02	0.88
1:H:271:LYS:CE	1:H:306:ARG:HG3	2.01	0.88
1:A:75:PRO:HG2	1:D:139:ASP:HB2	1.53	0.88
1:B:397:LEU:HD12	1:B:407:VAL:CG1	2.04	0.88
1:B:75:PRO:HG2	1:C:139:ASP:HB3	1.57	0.86
1:A:139:ASP:O	1:A:140:LEU:CD1	2.22	0.86
1:H:142:LEU:CB	1:H:143:PRO:HA	1.94	0.86
1:C:139:ASP:O	1:C:140:LEU:HD12	1.76	0.85
1:E:397:LEU:CD1	1:E:407:VAL:HG11	2.06	0.85
1:H:271:LYS:HG3	1:H:306:ARG:HE	1.40	0.85
1:A:362:ASP:CB	1:A:394:ILE:HG23	2.06	0.85
1:E:75:PRO:HG2	1:H:139:ASP:HB2	1.59	0.84
1:F:283:GLN:HG2	1:F:320:ARG:CD	2.07	0.84
1:H:140:LEU:HD11	1:H:152:ALA:HB2	1.59	0.84
1:B:142:LEU:HB2	1:B:143:PRO:HA	0.86	0.84
1:E:58:VAL:O	1:E:58:VAL:HG12	1.77	0.84
1:C:58:VAL:HG12	1:C:58:VAL:O	1.77	0.84
1:D:58:VAL:HG12	1:D:58:VAL:O	1.77	0.84
1:F:58:VAL:HG12	1:F:58:VAL:O	1.77	0.84
1:B:58:VAL:HG12	1:B:58:VAL:O	1.77	0.84
1:E:139:ASP:O	1:E:139:ASP:OD1	1.96	0.83
1:A:394:ILE:N	1:A:394:ILE:CD1	2.30	0.83
1:H:58:VAL:HG12	1:H:58:VAL:O	1.77	0.83
1:E:389:ARG:O	1:E:390:GLU:CB	2.27	0.83
1:A:114:MET:HE1	1:A:295:PHE:CZ	2.12	0.83
1:A:389:ARG:O	1:A:390:GLU:CB	2.27	0.83
1:A:142:LEU:HB2	1:A:143:PRO:CA	2.09	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:LEU:CD1	1:C:148:VAL:HG12	2.08	0.82
1:A:459:MET:HE3	1:B:144:LEU:HD21	1.59	0.82
1:F:389:ARG:O	1:F:390:GLU:CB	2.27	0.82
1:A:58:VAL:HG12	1:A:58:VAL:O	1.77	0.82
1:E:156:ARG:HG2	1:E:487:THR:HG21	1.61	0.82
1:A:122:TRP:CZ3	1:A:478:HIS:ND1	2.48	0.82
1:E:122:TRP:CZ3	1:E:478:HIS:ND1	2.48	0.81
1:E:142:LEU:HD22	1:F:459:MET:HB3	1.61	0.81
1:C:144:LEU:CD1	1:C:148:VAL:CG1	2.57	0.81
1:H:271:LYS:HE2	1:H:397:LEU:O	1.81	0.81
1:C:156:ARG:HG2	1:C:487:THR:HG21	1.61	0.81
1:G:58:VAL:HG12	1:G:58:VAL:O	1.77	0.81
1:B:371:THR:HG23	1:B:371:THR:O	1.78	0.81
1:H:166:ILE:HG12	1:H:193:PRO:HA	1.63	0.81
1:D:40:GLY:O	1:D:41:ASP:OD1	1.97	0.81
1:D:166:ILE:HG12	1:D:193:PRO:HA	1.63	0.81
1:B:51:VAL:HG22	1:B:231:ALA:HB2	1.63	0.81
1:E:51:VAL:HG22	1:E:231:ALA:HB2	1.63	0.81
1:E:166:ILE:HG12	1:E:193:PRO:HA	1.63	0.81
1:F:166:ILE:HG12	1:F:193:PRO:HA	1.63	0.81
1:F:51:VAL:HG22	1:F:231:ALA:HB2	1.63	0.80
1:F:139:ASP:HB2	1:G:75:PRO:HG2	1.61	0.80
1:G:166:ILE:HG12	1:G:193:PRO:HA	1.63	0.80
1:A:51:VAL:HG22	1:A:231:ALA:HB2	1.63	0.80
1:A:241:VAL:HG22	1:A:264:VAL:HG23	1.64	0.80
1:C:166:ILE:HG12	1:C:193:PRO:HA	1.63	0.80
1:E:65:LEU:HD21	1:E:160:GLY:HA2	1.64	0.80
1:B:166:ILE:HG12	1:B:193:PRO:HA	1.63	0.80
1:B:156:ARG:HG2	1:B:487:THR:HG21	1.61	0.80
1:B:293:ILE:HG13	1:B:293:ILE:O	1.81	0.80
1:H:293:ILE:HG13	1:H:293:ILE:O	1.81	0.80
1:C:51:VAL:HG22	1:C:231:ALA:HB2	1.63	0.80
1:D:51:VAL:HG22	1:D:231:ALA:HB2	1.63	0.80
1:D:293:ILE:HG13	1:D:293:ILE:O	1.81	0.80
1:G:51:VAL:HG22	1:G:231:ALA:HB2	1.63	0.80
1:E:139:ASP:O	1:E:140:LEU:CD2	2.30	0.79
1:D:65:LEU:HD11	1:D:160:GLY:HA2	1.65	0.79
1:E:140:LEU:CD1	1:E:152:ALA:CB	2.60	0.79
1:C:293:ILE:HG13	1:C:293:ILE:O	1.81	0.79
1:C:396:LEU:HD13	1:C:396:LEU:O	1.83	0.79
1:A:293:ILE:O	1:A:293:ILE:HG13	1.81	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:293:ILE:O	1:F:293:ILE:HG13	1.81	0.78
1:H:142:LEU:CB	1:H:143:PRO:CA	2.58	0.78
1:H:51:VAL:HG22	1:H:231:ALA:HB2	1.63	0.78
1:A:166:ILE:HG12	1:A:193:PRO:HA	1.63	0.78
1:B:425:VAL:O	1:B:471:ASP:HB2	1.84	0.78
1:E:293:ILE:HG13	1:E:293:ILE:O	1.81	0.78
1:G:139:ASP:O	1:G:140:LEU:CD2	2.23	0.78
1:C:65:LEU:HD11	1:C:160:GLY:HA2	1.66	0.78
1:C:425:VAL:O	1:C:471:ASP:HB2	1.84	0.77
1:B:397:LEU:HD11	1:B:407:VAL:HG11	1.60	0.77
1:G:293:ILE:O	1:G:293:ILE:HG13	1.82	0.77
1:G:425:VAL:O	1:G:471:ASP:HB2	1.83	0.77
1:G:65:LEU:HD21	1:G:160:GLY:HA2	1.67	0.77
1:D:425:VAL:O	1:D:471:ASP:HB2	1.84	0.77
1:F:425:VAL:O	1:F:471:ASP:HB2	1.84	0.77
1:E:80:ARG:HE	1:E:84:ARG:HE	1.33	0.77
1:A:156:ARG:HG2	1:A:487:THR:HG21	1.61	0.76
1:C:144:LEU:HD12	1:C:148:VAL:HG12	1.66	0.76
1:A:425:VAL:O	1:A:471:ASP:HB2	1.85	0.76
1:E:128:GLY:O	1:E:132:LYS:HD2	1.86	0.76
1:D:394:ILE:CD1	1:D:396:LEU:HB3	2.15	0.76
1:C:394:ILE:O	1:C:394:ILE:HG13	1.86	0.76
1:G:156:ARG:HG2	1:G:487:THR:HG21	1.61	0.76
1:B:142:LEU:CB	1:B:143:PRO:CA	2.45	0.76
1:D:64:THR:O	1:D:67:SER:HB2	1.86	0.76
1:D:128:GLY:O	1:D:132:LYS:HD2	1.86	0.76
1:G:128:GLY:O	1:G:132:LYS:HD2	1.86	0.75
1:F:394:ILE:O	1:F:395:ARG:CB	2.34	0.75
1:A:80:ARG:HE	1:A:84:ARG:HE	1.33	0.75
1:A:128:GLY:O	1:A:132:LYS:HD2	1.86	0.75
1:H:128:GLY:O	1:H:132:LYS:HD2	1.86	0.75
1:F:144:LEU:HD13	1:F:148:VAL:CG1	2.16	0.75
1:E:425:VAL:O	1:E:471:ASP:HB2	1.85	0.74
1:A:139:ASP:OD1	1:A:139:ASP:C	2.28	0.74
1:C:128:GLY:O	1:C:132:LYS:HD2	1.86	0.74
1:C:139:ASP:O	1:C:140:LEU:CD1	2.36	0.74
1:F:64:THR:O	1:F:64:THR:HG22	1.87	0.74
1:H:64:THR:O	1:H:67:SER:HB2	1.86	0.74
1:B:64:THR:HG22	1:B:64:THR:O	1.87	0.73
1:B:397:LEU:HD11	1:B:407:VAL:CG1	2.13	0.73
1:F:296:ASN:ND2	1:F:299:GLN:O	2.20	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:483:ILE:HG22	1:D:483:ILE:O	1.89	0.72
1:D:394:ILE:HD11	1:D:396:LEU:HB3	1.71	0.72
1:H:483:ILE:O	1:H:483:ILE:HG22	1.89	0.72
1:E:296:ASN:ND2	1:E:299:GLN:O	2.23	0.71
1:H:142:LEU:HD13	1:H:144:LEU:HG	1.72	0.71
1:C:144:LEU:CB	1:C:148:VAL:HG11	2.20	0.71
1:F:144:LEU:CD1	1:F:148:VAL:HG12	2.21	0.70
1:H:65:LEU:HD11	1:H:160:GLY:HA2	1.73	0.70
1:H:389:ARG:O	1:H:390:GLU:CB	2.40	0.70
1:A:58:VAL:O	1:A:58:VAL:CG1	2.40	0.70
1:H:144:LEU:HB3	1:H:145:PRO:HD2	1.74	0.70
1:D:58:VAL:O	1:D:58:VAL:CG1	2.40	0.69
1:C:58:VAL:O	1:C:58:VAL:CG1	2.40	0.69
1:G:58:VAL:O	1:G:58:VAL:CG1	2.40	0.69
1:B:58:VAL:O	1:B:58:VAL:CG1	2.40	0.69
1:A:428:LEU:HD12	1:A:468:GLY:HA3	1.74	0.69
1:C:144:LEU:HB3	1:C:148:VAL:CG1	2.22	0.69
1:D:389:ARG:O	1:D:390:GLU:CB	2.40	0.69
1:E:146:PRO:O	1:E:147:GLU:CB	2.41	0.69
1:F:144:LEU:HD13	1:F:148:VAL:HG12	1.74	0.69
1:E:142:LEU:HB2	1:E:143:PRO:CA	2.22	0.68
1:E:122:TRP:CZ3	1:E:478:HIS:CE1	2.81	0.68
1:H:58:VAL:O	1:H:58:VAL:CG1	2.40	0.68
1:F:58:VAL:O	1:F:58:VAL:CG1	2.40	0.68
1:H:80:ARG:HH11	1:H:80:ARG:HG3	1.59	0.68
1:E:142:LEU:HB2	1:E:143:PRO:HA	1.75	0.68
1:D:441:LEU:O	1:D:444:ASN:HB3	1.93	0.68
1:B:157:VAL:O	1:B:487:THR:HG23	1.94	0.68
1:F:139:ASP:C	1:F:140:LEU:HG	2.19	0.68
1:A:122:TRP:CZ3	1:A:478:HIS:CE1	2.81	0.68
1:D:80:ARG:HG3	1:D:80:ARG:HH11	1.58	0.68
1:E:140:LEU:CD1	1:E:152:ALA:HB2	2.24	0.68
1:C:157:VAL:O	1:C:487:THR:HG23	1.94	0.68
1:F:247:THR:HA	1:F:268:LEU:HB3	1.76	0.68
1:G:170:PHE:CE1	1:G:296:ASN:ND2	2.62	0.68
1:C:140:LEU:HD23	1:C:142:LEU:HD21	1.74	0.68
1:C:156:ARG:CG	1:C:487:THR:CG2	2.50	0.68
1:F:397:LEU:CD1	1:F:407:VAL:HG11	2.24	0.68
1:A:247:THR:HA	1:A:268:LEU:HB3	1.76	0.67
1:C:247:THR:HA	1:C:268:LEU:HB3	1.76	0.67
1:H:441:LEU:O	1:H:444:ASN:HB3	1.93	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:VAL:O	1:A:487:THR:HG23	1.94	0.67
1:G:157:VAL:O	1:G:487:THR:HG23	1.94	0.67
1:G:247:THR:HA	1:G:268:LEU:HB3	1.76	0.67
1:E:157:VAL:O	1:E:487:THR:HG23	1.94	0.67
1:F:144:LEU:HB3	1:F:145:PRO:HD2	1.76	0.67
1:E:247:THR:HA	1:E:268:LEU:HB3	1.76	0.67
1:B:437:LEU:HD11	1:B:441:LEU:HD11	1.77	0.66
1:B:496:TYR:CD2	1:D:441:LEU:HD23	2.30	0.66
1:E:58:VAL:O	1:E:58:VAL:CG1	2.40	0.66
1:F:496:TYR:CD2	1:H:441:LEU:HD23	2.30	0.66
1:E:79:GLU:O	1:E:83:LEU:CD1	2.38	0.66
1:E:80:ARG:NE	1:E:84:ARG:HE	1.93	0.66
1:G:389:ARG:O	1:G:390:GLU:CB	2.44	0.66
1:H:247:THR:HA	1:H:268:LEU:HB3	1.76	0.66
1:G:170:PHE:HB2	1:G:174:MET:HG2	1.78	0.66
1:A:357:ARG:O	1:A:361:GLU:HG3	1.94	0.66
1:A:393:ASP:C	1:A:394:ILE:O	2.28	0.66
1:E:118:ALA:O	1:E:122:TRP:CD1	2.42	0.66
1:A:118:ALA:O	1:A:122:TRP:CD1	2.42	0.66
1:D:247:THR:HA	1:D:268:LEU:HB3	1.76	0.66
1:E:140:LEU:HD11	1:E:152:ALA:HB3	1.78	0.66
1:B:156:ARG:CG	1:B:487:THR:CG2	2.50	0.66
1:E:437:LEU:HD11	1:E:441:LEU:HD11	1.77	0.66
1:F:142:LEU:HB2	1:F:143:PRO:CA	2.21	0.66
1:G:64:THR:O	1:G:67:SER:HB3	1.96	0.66
1:H:474:VAL:O	1:H:474:VAL:HG23	1.96	0.66
1:A:80:ARG:NE	1:A:84:ARG:HE	1.93	0.65
1:C:64:THR:O	1:C:67:SER:HB3	1.96	0.65
1:A:397:LEU:CD1	1:A:407:VAL:CG1	2.65	0.65
1:G:474:VAL:HG23	1:G:474:VAL:O	1.97	0.65
1:H:271:LYS:HZ2	1:H:305:SER:HB2	1.61	0.65
1:D:170:PHE:CE1	1:D:296:ASN:ND2	2.64	0.65
1:A:487:THR:HG22	1:A:488:THR:N	2.12	0.65
1:E:140:LEU:HD12	1:E:152:ALA:HB2	1.78	0.65
1:H:84:ARG:HG3	1:H:84:ARG:HH11	1.62	0.65
1:H:271:LYS:HG3	1:H:306:ARG:NE	2.10	0.65
1:D:144:LEU:HB3	1:D:145:PRO:HD2	1.79	0.64
1:D:140:LEU:HD23	1:D:142:LEU:HD21	1.79	0.64
1:A:428:LEU:HD12	1:A:468:GLY:CA	2.26	0.64
1:F:139:ASP:O	1:F:140:LEU:CD2	2.45	0.64
1:B:474:VAL:HG23	1:B:474:VAL:O	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:LEU:CB	1:C:148:VAL:CG1	2.75	0.64
1:C:493:VAL:HG21	1:D:464:LEU:HD11	1.79	0.64
1:G:487:THR:HG22	1:G:488:THR:N	2.12	0.64
1:D:474:VAL:HG23	1:D:474:VAL:O	1.96	0.64
1:E:467:GLY:HA3	1:E:476:ARG:HD3	1.78	0.64
1:G:493:VAL:HG21	1:H:464:LEU:HD11	1.79	0.64
1:B:128:GLY:O	1:B:132:LYS:HD2	1.97	0.64
1:C:413:ASP:OD1	1:C:416:GLU:CG	2.44	0.64
1:D:84:ARG:HG3	1:D:84:ARG:HH11	1.62	0.64
1:F:128:GLY:O	1:F:132:LYS:HD2	1.97	0.64
1:A:467:GLY:HA3	1:A:476:ARG:HD3	1.78	0.64
1:E:474:VAL:HG23	1:E:474:VAL:O	1.97	0.64
1:B:467:GLY:HA3	1:B:476:ARG:HD3	1.80	0.63
1:C:487:THR:HG22	1:C:488:THR:N	2.12	0.63
1:E:487:THR:HG22	1:E:488:THR:N	2.11	0.63
1:H:271:LYS:NZ	1:H:305:SER:HB2	2.13	0.63
1:D:139:ASP:OD1	1:D:139:ASP:C	2.41	0.63
1:D:467:GLY:HA3	1:D:476:ARG:HD3	1.80	0.63
1:E:277:LEU:HD12	1:E:434:THR:OG1	1.98	0.63
1:A:277:LEU:HD12	1:A:434:THR:OG1	1.98	0.63
1:B:426:TYR:HB3	1:B:472:SER:OG	1.98	0.63
1:A:474:VAL:HG23	1:A:474:VAL:O	1.97	0.63
1:A:142:LEU:HD13	1:A:144:LEU:HG	1.80	0.63
1:C:365:ASP:HB3	1:C:387:ALA:HB3	1.80	0.63
1:B:487:THR:HG22	1:B:488:THR:N	2.12	0.63
1:G:365:ASP:HB3	1:G:387:ALA:HB3	1.80	0.63
1:F:474:VAL:HG23	1:F:474:VAL:O	1.97	0.63
1:B:277:LEU:HD12	1:B:434:THR:OG1	1.98	0.63
1:B:39:THR:O	1:B:41:ASP:N	2.31	0.62
1:F:277:LEU:HD12	1:F:434:THR:OG1	1.98	0.62
1:H:467:GLY:HA3	1:H:476:ARG:HD3	1.81	0.62
1:H:396:LEU:HD23	1:H:407:VAL:CB	2.21	0.62
1:C:467:GLY:HA3	1:C:476:ARG:HD3	1.81	0.62
1:E:394:ILE:CG2	1:E:394:ILE:O	2.47	0.62
1:F:467:GLY:HA3	1:F:476:ARG:HD3	1.80	0.62
1:E:139:ASP:O	1:E:140:LEU:CG	2.47	0.62
1:A:397:LEU:HD11	1:A:407:VAL:HG11	1.78	0.62
1:B:396:LEU:HD13	1:B:396:LEU:O	1.99	0.62
1:A:139:ASP:O	1:A:139:ASP:OD1	2.17	0.62
1:A:142:LEU:CB	1:A:143:PRO:HA	2.11	0.62
1:A:241:VAL:HG22	1:A:241:VAL:O	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:LEU:CD1	1:D:160:GLY:HA2	2.30	0.62
1:G:467:GLY:HA3	1:G:476:ARG:HD3	1.80	0.62
1:H:389:ARG:HG2	1:H:389:ARG:HH11	1.65	0.62
1:A:139:ASP:O	1:A:140:LEU:HD13	2.00	0.61
1:B:247:THR:HA	1:B:268:LEU:HB3	1.81	0.61
1:D:389:ARG:HG2	1:D:389:ARG:HH11	1.65	0.61
1:C:474:VAL:O	1:C:474:VAL:HG13	1.99	0.61
1:E:394:ILE:O	1:E:395:ARG:CB	2.46	0.61
1:B:125:TYR:CD1	1:D:131:THR:CG2	2.84	0.61
1:C:65:LEU:CD1	1:C:160:GLY:HA2	2.30	0.61
1:B:125:TYR:CD1	1:D:131:THR:HG23	2.36	0.61
1:F:142:LEU:CB	1:F:143:PRO:HA	2.25	0.61
1:F:125:TYR:CD1	1:H:131:THR:CG2	2.84	0.60
1:A:79:GLU:O	1:A:83:LEU:CD1	2.38	0.60
1:D:137:THR:O	1:D:137:THR:HG22	2.01	0.60
1:E:180:ALA:HB3	1:E:181:PRO:CD	2.32	0.60
1:F:395:ARG:C	1:F:397:LEU:H	2.08	0.60
1:H:442:ARG:HA	1:H:445:ASP:HB2	1.83	0.60
1:A:368:CYS:O	1:A:384:THR:HA	2.02	0.60
1:A:397:LEU:HD12	1:A:407:VAL:CG1	2.22	0.60
1:D:142:LEU:HD13	1:D:144:LEU:HG	1.83	0.60
1:H:192:LYS:HE3	1:H:225:GLY:HA2	1.84	0.60
1:A:180:ALA:HB3	1:A:181:PRO:CD	2.32	0.60
1:A:242:ALA:HA	1:A:265:SER:HB3	1.84	0.60
1:C:180:ALA:HB3	1:C:181:PRO:CD	2.32	0.60
1:D:180:ALA:HB3	1:D:181:PRO:CD	2.32	0.60
1:E:156:ARG:CG	1:E:487:THR:CG2	2.50	0.60
1:B:180:ALA:HB3	1:B:181:PRO:CD	2.32	0.60
1:H:65:LEU:CD1	1:H:160:GLY:HA2	2.32	0.60
1:B:297:HIS:N	1:B:297:HIS:CD2	2.69	0.60
1:D:426:TYR:HB3	1:D:472:SER:OG	2.01	0.59
1:H:146:PRO:O	1:H:147:GLU:CB	2.50	0.59
1:H:137:THR:HG22	1:H:137:THR:O	2.01	0.59
1:C:242:ALA:HA	1:C:265:SER:HB3	1.84	0.59
1:F:180:ALA:HB3	1:F:181:PRO:CD	2.32	0.59
1:C:146:PRO:O	1:C:147:GLU:C	2.37	0.59
1:C:459:MET:HE3	1:D:144:LEU:HD21	1.83	0.59
1:E:242:ALA:HA	1:E:265:SER:HB3	1.84	0.59
1:F:125:TYR:CD1	1:H:131:THR:HG23	2.36	0.59
1:D:146:PRO:O	1:D:147:GLU:CB	2.50	0.59
1:G:242:ALA:HA	1:G:265:SER:HB3	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:VAL:HG21	1:A:253:ILE:CG2	2.33	0.59
1:F:151:ARG:HG2	1:F:496:TYR:HE2	1.68	0.59
1:G:156:ARG:CG	1:G:487:THR:CG2	2.50	0.59
1:E:142:LEU:N	1:E:143:PRO:HA	2.16	0.59
1:G:180:ALA:HB3	1:G:181:PRO:CD	2.32	0.59
1:H:180:ALA:HB3	1:H:181:PRO:CD	2.32	0.59
1:F:80:ARG:O	1:F:84:ARG:HG3	2.03	0.59
1:F:297:HIS:N	1:F:297:HIS:CD2	2.69	0.59
1:H:142:LEU:CD1	1:H:144:LEU:HG	2.31	0.59
1:A:139:ASP:CB	1:D:75:PRO:HG2	2.27	0.58
1:B:151:ARG:HG2	1:B:496:TYR:HE2	1.68	0.58
1:F:242:ALA:HA	1:F:265:SER:HB3	1.84	0.58
1:G:454:VAL:HB	1:H:494:ILE:HG23	1.84	0.58
1:B:80:ARG:O	1:B:84:ARG:HG3	2.03	0.58
1:B:242:ALA:HA	1:B:265:SER:HB3	1.84	0.58
1:G:277:LEU:HD12	1:G:434:THR:OG1	2.03	0.58
1:C:454:VAL:HB	1:D:494:ILE:HG23	1.84	0.58
1:E:142:LEU:HB3	1:F:459:MET:SD	2.43	0.58
1:C:142:LEU:HD13	1:C:144:LEU:HG	1.86	0.58
1:C:144:LEU:HB3	1:C:145:PRO:HD2	1.86	0.58
1:C:277:LEU:HD12	1:C:434:THR:OG1	2.03	0.58
1:F:140:LEU:CD1	1:F:152:ALA:HB2	2.11	0.58
1:E:113:LEU:N	1:E:113:LEU:HD23	2.18	0.57
1:D:142:LEU:CB	1:D:143:PRO:CA	2.66	0.57
1:F:144:LEU:HB3	1:F:145:PRO:CD	2.34	0.57
1:A:140:LEU:HG	1:B:461:ASP:HB2	1.87	0.57
1:A:477:GLU:HG3	1:A:478:HIS:CE1	2.38	0.57
1:E:101:THR:HG21	1:E:334:LEU:HG	1.86	0.57
1:B:101:THR:HG21	1:B:334:LEU:HG	1.86	0.57
1:C:101:THR:HG21	1:C:334:LEU:HG	1.86	0.57
1:D:397:LEU:HD23	1:D:407:VAL:HG11	1.86	0.57
1:H:396:LEU:CG	1:H:407:VAL:HB	2.34	0.57
1:A:17:MET:HE2	1:A:47:PRO:HB2	1.87	0.57
1:H:144:LEU:HB3	1:H:145:PRO:CD	2.35	0.57
1:E:365:ASP:HB3	1:E:387:ALA:HB3	1.86	0.57
1:F:64:THR:O	1:F:64:THR:CG2	2.51	0.57
1:H:247:THR:HG21	1:H:426:TYR:OH	2.05	0.56
1:B:151:ARG:HG2	1:B:496:TYR:CE2	2.41	0.56
1:C:296:ASN:ND2	1:C:299:GLN:O	2.34	0.56
1:F:281:ASP:HB3	1:F:284:GLU:HB2	1.87	0.56
1:H:17:MET:HE2	1:H:47:PRO:HB3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LEU:CB	1:A:143:PRO:CA	2.77	0.56
1:A:365:ASP:HB3	1:A:387:ALA:HB3	1.86	0.56
1:E:247:THR:HG21	1:E:426:TYR:OH	2.06	0.56
1:C:146:PRO:O	1:C:147:GLU:CB	2.50	0.56
1:F:365:ASP:HB2	1:F:387:ALA:HB3	1.88	0.56
1:H:101:THR:HG21	1:H:334:LEU:HG	1.87	0.56
1:C:277:LEU:HD12	1:C:434:THR:CB	2.36	0.56
1:F:139:ASP:C	1:F:139:ASP:OD1	2.46	0.56
1:G:260:SER:HB3	1:G:262:LYS:HE3	1.88	0.56
1:D:17:MET:HE2	1:D:47:PRO:HB3	1.87	0.56
1:D:296:ASN:ND2	1:D:299:GLN:O	2.39	0.56
1:D:427:GLY:O	1:D:449:ALA:HA	2.06	0.56
1:E:260:SER:HB3	1:E:262:LYS:HE3	1.88	0.56
1:A:75:PRO:HG2	1:D:139:ASP:CB	2.31	0.56
1:A:241:VAL:O	1:A:241:VAL:CG2	2.53	0.56
1:D:389:ARG:HG2	1:D:389:ARG:NH1	2.21	0.56
1:G:277:LEU:HD12	1:G:434:THR:CB	2.36	0.56
1:H:260:SER:HB3	1:H:262:LYS:HE3	1.88	0.56
1:B:18:LEU:HD22	1:B:205:ALA:HB1	1.88	0.56
1:B:64:THR:O	1:B:64:THR:CG2	2.51	0.56
1:C:260:SER:HB3	1:C:262:LYS:HE3	1.88	0.56
1:D:101:THR:HG21	1:D:334:LEU:HG	1.86	0.56
1:F:151:ARG:HG2	1:F:496:TYR:CE2	2.40	0.56
1:G:101:THR:HG21	1:G:334:LEU:HG	1.86	0.56
1:H:84:ARG:HG3	1:H:84:ARG:NH1	2.21	0.56
1:A:149:ARG:NH1	1:C:445:ASP:OD1	2.39	0.55
1:E:140:LEU:CD1	1:E:152:ALA:HB3	2.34	0.55
1:F:260:SER:HB3	1:F:262:LYS:HE3	1.88	0.55
1:C:18:LEU:HD22	1:C:205:ALA:HB1	1.88	0.55
1:D:84:ARG:HG3	1:D:84:ARG:NH1	2.21	0.55
1:D:260:SER:HB3	1:D:262:LYS:HE3	1.88	0.55
1:E:17:MET:HE2	1:E:47:PRO:HB2	1.87	0.55
1:A:397:LEU:HD11	1:A:407:VAL:CG1	2.35	0.55
1:A:144:LEU:HB3	1:A:145:PRO:HD2	1.88	0.55
1:A:146:PRO:C	1:A:148:VAL:H	2.14	0.55
1:B:369:GLY:HA3	1:B:384:THR:HA	1.88	0.55
1:F:18:LEU:HD22	1:F:205:ALA:HB1	1.88	0.55
1:F:494:ILE:HG21	1:H:437:LEU:HD21	1.87	0.55
1:G:18:LEU:HD22	1:G:205:ALA:HB1	1.88	0.55
1:E:139:ASP:OD1	1:E:139:ASP:C	2.48	0.55
1:H:271:LYS:HE3	1:H:306:ARG:HG2	1.79	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:ASP:HB2	1:B:387:ALA:HB3	1.88	0.55
1:E:135:GLY:H	1:H:137:THR:HG22	1.71	0.55
1:E:144:LEU:CB	1:E:145:PRO:CD	2.73	0.55
1:H:140:LEU:HD11	1:H:152:ALA:CB	2.35	0.55
1:B:140:LEU:HD23	1:B:142:LEU:HD21	1.89	0.55
1:D:18:LEU:HD22	1:D:205:ALA:HB1	1.88	0.55
1:D:394:ILE:HD12	1:D:396:LEU:HB3	1.87	0.55
1:H:18:LEU:HD22	1:H:205:ALA:HB1	1.88	0.55
1:B:40:GLY:O	1:B:41:ASP:OD1	2.24	0.55
1:C:145:PRO:O	1:C:148:VAL:HB	2.07	0.55
1:A:135:GLY:H	1:D:137:THR:HG22	1.71	0.54
1:A:393:ASP:CG	1:A:393:ASP:O	2.50	0.54
1:E:65:LEU:CD2	1:E:160:GLY:HA2	2.35	0.54
1:A:260:SER:HB3	1:A:262:LYS:HE3	1.88	0.54
1:B:260:SER:HB3	1:B:262:LYS:HE3	1.88	0.54
1:G:65:LEU:CD2	1:G:160:GLY:HA2	2.37	0.54
1:C:142:LEU:CB	1:C:143:PRO:CA	2.61	0.54
1:E:39:THR:OG1	1:E:41:ASP:OD1	2.25	0.54
1:H:389:ARG:HG2	1:H:389:ARG:NH1	2.21	0.54
1:E:112:LYS:C	1:E:113:LEU:HD23	2.32	0.54
1:B:281:ASP:OD2	1:B:284:GLU:HG3	2.08	0.53
1:E:394:ILE:O	1:E:394:ILE:HG22	2.08	0.53
1:F:17:MET:HG2	1:F:47:PRO:HG2	1.88	0.53
1:C:389:ARG:O	1:C:390:GLU:CB	2.56	0.53
1:C:413:ASP:OD1	1:C:416:GLU:HB3	2.09	0.53
1:G:396:LEU:HD13	1:G:396:LEU:O	2.09	0.53
1:C:36:ASN:C	1:C:36:ASN:OD1	2.51	0.53
1:D:131:THR:HG22	1:D:132:LYS:NZ	2.24	0.53
1:F:23:TRP:HZ2	1:F:206:GLU:HB3	1.74	0.53
1:G:36:ASN:OD1	1:G:36:ASN:C	2.51	0.53
1:B:348:HIS:HE1	1:B:402:PHE:HB3	1.74	0.53
1:B:125:TYR:CE1	1:D:131:THR:HG23	2.44	0.53
1:F:348:HIS:HE1	1:F:402:PHE:HB3	1.74	0.53
1:G:348:HIS:HE1	1:G:402:PHE:HB3	1.74	0.53
1:H:271:LYS:HG2	1:H:397:LEU:O	2.08	0.53
1:H:277:LEU:HD12	1:H:434:THR:OG1	2.09	0.53
1:C:146:PRO:O	1:C:148:VAL:HG23	2.08	0.52
1:C:494:ILE:HG23	1:D:454:VAL:HB	1.92	0.52
1:D:23:TRP:HZ2	1:D:206:GLU:HB3	1.74	0.52
1:F:395:ARG:C	1:F:397:LEU:N	2.63	0.52
1:G:23:TRP:HZ2	1:G:206:GLU:HB3	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:139:ASP:C	1:G:140:LEU:HD23	2.22	0.52
1:H:131:THR:HG22	1:H:132:LYS:NZ	2.24	0.52
1:B:394:ILE:HG13	1:B:396:LEU:H	1.74	0.52
1:A:156:ARG:CG	1:A:487:THR:CG2	2.50	0.52
1:A:316:ASP:O	1:A:320:ARG:HG3	2.10	0.52
1:B:125:TYR:C	1:B:125:TYR:CD2	2.87	0.52
1:D:20:GLY:O	1:F:376:ALA:HB2	2.10	0.52
1:F:125:TYR:CD2	1:F:125:TYR:C	2.87	0.52
1:G:283:GLN:OE1	1:G:320:ARG:HD3	2.09	0.52
1:H:483:ILE:O	1:H:483:ILE:CG2	2.57	0.52
1:A:125:TYR:C	1:A:125:TYR:CD2	2.87	0.52
1:C:316:ASP:O	1:C:320:ARG:HG3	2.10	0.52
1:E:23:TRP:HZ2	1:E:206:GLU:HB3	1.74	0.52
1:F:125:TYR:CE1	1:H:131:THR:HG23	2.44	0.52
1:G:125:TYR:C	1:G:125:TYR:CD2	2.88	0.52
1:H:125:TYR:C	1:H:125:TYR:CD2	2.88	0.52
1:H:316:ASP:O	1:H:320:ARG:HG3	2.10	0.52
1:B:23:TRP:HZ2	1:B:206:GLU:HB3	1.74	0.52
1:D:277:LEU:HD12	1:D:434:THR:OG1	2.09	0.52
1:F:316:ASP:O	1:F:320:ARG:HG3	2.10	0.52
1:F:394:ILE:O	1:F:394:ILE:HG22	2.10	0.52
1:G:297:HIS:N	1:G:297:HIS:CD2	2.78	0.52
1:G:494:ILE:HG23	1:H:454:VAL:HB	1.91	0.52
1:H:277:LEU:HD12	1:H:434:THR:CB	2.40	0.52
1:B:119:SER:HB3	1:B:176:VAL:HG21	1.92	0.52
1:C:125:TYR:C	1:C:125:TYR:CD2	2.88	0.52
1:C:297:HIS:CD2	1:C:297:HIS:N	2.78	0.52
1:H:23:TRP:HZ2	1:H:206:GLU:HB3	1.74	0.52
1:A:23:TRP:HZ2	1:A:206:GLU:HB3	1.74	0.52
1:B:316:ASP:O	1:B:320:ARG:HG3	2.10	0.52
1:D:144:LEU:HB3	1:D:145:PRO:CD	2.40	0.52
1:A:168:TRP:CE3	1:A:344:VAL:HG21	2.45	0.52
1:B:140:LEU:HG	1:B:142:LEU:HD21	1.90	0.52
1:D:297:HIS:CD2	1:D:297:HIS:N	2.78	0.52
1:E:296:ASN:O	1:E:299:GLN:HB2	2.10	0.52
1:E:316:ASP:O	1:E:320:ARG:HG3	2.10	0.52
1:F:348:HIS:CE1	1:F:402:PHE:HB3	2.45	0.52
1:H:348:HIS:CE1	1:H:402:PHE:HB3	2.45	0.52
1:B:348:HIS:CE1	1:B:402:PHE:HB3	2.45	0.52
1:C:51:VAL:HG12	1:C:51:VAL:O	2.10	0.52
1:D:348:HIS:HE1	1:D:402:PHE:HB3	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:TYR:C	1:E:125:TYR:CD2	2.87	0.52
1:C:23:TRP:HZ2	1:C:206:GLU:HB3	1.74	0.52
1:C:168:TRP:CE3	1:C:344:VAL:HG21	2.45	0.52
1:E:348:HIS:HE1	1:E:402:PHE:HB3	1.74	0.52
1:G:296:ASN:O	1:G:299:GLN:HB2	2.10	0.52
1:H:348:HIS:HE1	1:H:402:PHE:HB3	1.74	0.52
1:B:51:VAL:HG12	1:B:51:VAL:O	2.10	0.51
1:F:168:TRP:CE3	1:F:344:VAL:HG21	2.45	0.51
1:G:316:ASP:O	1:G:320:ARG:HG3	2.10	0.51
1:A:348:HIS:HE1	1:A:402:PHE:HB3	1.74	0.51
1:C:39:THR:O	1:C:41:ASP:N	2.44	0.51
1:D:348:HIS:CE1	1:D:402:PHE:HB3	2.45	0.51
1:B:168:TRP:CE3	1:B:344:VAL:HG21	2.45	0.51
1:G:168:TRP:CE3	1:G:344:VAL:HG21	2.45	0.51
1:H:227:THR:OG1	1:H:228:ALA:N	2.43	0.51
1:A:297:HIS:CD2	1:A:297:HIS:N	2.78	0.51
1:C:459:MET:HE3	1:D:144:LEU:CD2	2.40	0.51
1:D:125:TYR:CD2	1:D:125:TYR:C	2.87	0.51
1:E:168:TRP:CE3	1:E:344:VAL:HG21	2.45	0.51
1:F:46:VAL:CG1	1:F:47:PRO:HD2	2.41	0.51
1:A:348:HIS:CE1	1:A:402:PHE:HB3	2.45	0.51
1:B:46:VAL:CG1	1:B:47:PRO:HD2	2.41	0.51
1:C:348:HIS:CE1	1:C:402:PHE:HB3	2.45	0.51
1:C:296:ASN:O	1:C:299:GLN:HB2	2.10	0.51
1:C:394:ILE:O	1:C:394:ILE:CG1	2.58	0.51
1:D:316:ASP:O	1:D:320:ARG:HG3	2.10	0.51
1:E:426:TYR:CE1	1:E:471:ASP:HB3	2.46	0.51
1:D:168:TRP:CE3	1:D:344:VAL:HG21	2.45	0.51
1:G:46:VAL:CG1	1:G:47:PRO:HD2	2.40	0.51
1:G:348:HIS:CE1	1:G:402:PHE:HB3	2.45	0.51
1:C:348:HIS:HE1	1:C:402:PHE:HB3	1.74	0.51
1:D:296:ASN:O	1:D:299:GLN:HB2	2.10	0.51
1:E:321:LEU:HG	1:E:385:ILE:HD13	1.93	0.51
1:H:168:TRP:CE3	1:H:344:VAL:HG21	2.45	0.51
1:C:46:VAL:CG1	1:C:47:PRO:HD2	2.41	0.51
1:D:277:LEU:HD12	1:D:434:THR:CB	2.40	0.51
1:H:131:THR:HG22	1:H:132:LYS:HZ2	1.76	0.51
1:E:140:LEU:HD12	1:E:152:ALA:CB	2.37	0.51
1:F:119:SER:HB3	1:F:176:VAL:HG21	1.92	0.51
1:H:297:HIS:N	1:H:297:HIS:CD2	2.78	0.51
1:A:51:VAL:HG12	1:A:51:VAL:O	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:ASN:OD1	1:C:435:ASN:O	2.29	0.50
1:C:254:GLY:HA3	1:D:258:GLY:O	2.11	0.50
1:D:51:VAL:HG12	1:D:51:VAL:O	2.10	0.50
1:E:149:ARG:NH1	1:G:445:ASP:OD1	2.44	0.50
1:E:434:THR:HG21	1:E:440:ALA:HB2	1.93	0.50
1:F:321:LEU:HG	1:F:385:ILE:HD13	1.93	0.50
1:H:51:VAL:HG12	1:H:51:VAL:O	2.10	0.50
1:H:435:ASN:OD1	1:H:435:ASN:O	2.30	0.50
1:A:114:MET:CE	1:A:295:PHE:HE1	2.14	0.50
1:B:474:VAL:O	1:B:474:VAL:CG2	2.60	0.50
1:D:67:SER:OG	1:D:69:THR:HG22	2.12	0.50
1:E:139:ASP:C	1:E:140:LEU:HG	2.37	0.50
1:C:397:LEU:HD23	1:C:407:VAL:HG11	1.92	0.50
1:E:348:HIS:CE1	1:E:402:PHE:HB3	2.45	0.50
1:A:321:LEU:HG	1:A:385:ILE:HD13	1.93	0.50
1:A:434:THR:HG21	1:A:440:ALA:HB2	1.94	0.50
1:B:293:ILE:O	1:B:293:ILE:CG1	2.56	0.50
1:D:435:ASN:OD1	1:D:435:ASN:O	2.30	0.50
1:F:434:THR:HG21	1:F:440:ALA:HB2	1.93	0.50
1:D:446:GLU:HA	1:D:446:GLU:OE1	2.12	0.50
1:F:139:ASP:O	1:F:140:LEU:HD23	2.10	0.50
1:A:45:GLU:C	1:A:46:VAL:HG23	2.37	0.50
1:B:79:GLU:O	1:B:83:LEU:HG	2.12	0.50
1:C:274:VAL:HG22	1:C:307:LEU:CD1	2.42	0.50
1:E:297:HIS:CD2	1:E:297:HIS:N	2.78	0.50
1:F:144:LEU:HD12	1:F:148:VAL:HG12	1.93	0.50
1:F:474:VAL:O	1:F:474:VAL:CG2	2.60	0.50
1:G:435:ASN:OD1	1:G:435:ASN:O	2.29	0.50
1:G:446:GLU:OE1	1:G:446:GLU:HA	2.12	0.50
1:A:274:VAL:HG22	1:A:307:LEU:CD1	2.42	0.50
1:A:446:GLU:HA	1:A:446:GLU:OE1	2.12	0.50
1:B:107:LEU:HD21	1:B:338:VAL:HG12	1.94	0.50
1:B:274:VAL:HG22	1:B:307:LEU:CD1	2.42	0.50
1:B:283:GLN:OE1	1:B:320:ARG:NH1	2.36	0.50
1:B:321:LEU:HG	1:B:385:ILE:HD13	1.93	0.50
1:E:45:GLU:C	1:E:46:VAL:HG23	2.37	0.50
1:E:396:LEU:HD21	1:E:401:VAL:HG21	1.94	0.50
1:G:51:VAL:HG12	1:G:51:VAL:O	2.10	0.50
1:G:274:VAL:HG22	1:G:307:LEU:CD1	2.42	0.50
1:A:45:GLU:O	1:A:46:VAL:CG2	2.60	0.50
1:C:144:LEU:C	1:C:145:PRO:O	2.54	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:274:VAL:HG22	1:E:307:LEU:CD1	2.42	0.50
1:F:51:VAL:O	1:F:51:VAL:HG12	2.10	0.50
1:F:107:LEU:HD21	1:F:338:VAL:HG12	1.94	0.50
1:H:446:GLU:OE1	1:H:446:GLU:HA	2.12	0.50
1:A:393:ASP:O	1:A:393:ASP:OD1	2.29	0.49
1:B:446:GLU:OE1	1:B:446:GLU:HA	2.12	0.49
1:C:446:GLU:OE1	1:C:446:GLU:HA	2.12	0.49
1:D:425:VAL:HG12	1:D:426:TYR:CZ	2.47	0.49
1:F:274:VAL:HG22	1:F:307:LEU:CD1	2.42	0.49
1:A:22:GLN:O	1:A:24:VAL:HG23	2.12	0.49
1:B:140:LEU:CG	1:B:142:LEU:HD21	2.41	0.49
1:C:107:LEU:HD21	1:C:338:VAL:HG12	1.94	0.49
1:F:144:LEU:HD13	1:F:148:VAL:HG11	1.93	0.49
1:H:274:VAL:HG22	1:H:307:LEU:CD1	2.42	0.49
1:B:434:THR:HG21	1:B:440:ALA:HB2	1.94	0.49
1:D:23:TRP:CZ2	1:D:206:GLU:HB3	2.48	0.49
1:D:80:ARG:HH11	1:D:80:ARG:CG	2.24	0.49
1:G:254:GLY:HA3	1:H:258:GLY:O	2.11	0.49
1:G:321:LEU:HG	1:G:385:ILE:HD13	1.93	0.49
1:B:23:TRP:CZ2	1:B:206:GLU:HB3	2.48	0.49
1:C:321:LEU:HG	1:C:385:ILE:HD13	1.93	0.49
1:D:425:VAL:HG12	1:D:426:TYR:CE2	2.48	0.49
1:E:446:GLU:OE1	1:E:446:GLU:HA	2.12	0.49
1:F:79:GLU:O	1:F:83:LEU:HG	2.12	0.49
1:F:446:GLU:HA	1:F:446:GLU:OE1	2.12	0.49
1:G:107:LEU:HD21	1:G:338:VAL:HG12	1.94	0.49
1:C:493:VAL:CG2	1:D:464:LEU:HD11	2.43	0.49
1:D:274:VAL:HG22	1:D:307:LEU:CD1	2.42	0.49
1:E:51:VAL:HG12	1:E:51:VAL:O	2.10	0.49
1:G:16:GLN:OE1	1:G:23:TRP:HB3	2.13	0.49
1:A:107:LEU:HD21	1:A:338:VAL:HG12	1.94	0.49
1:E:142:LEU:HB2	1:E:143:PRO:C	2.38	0.49
1:E:142:LEU:H	1:E:143:PRO:HA	1.76	0.49
1:G:474:VAL:O	1:G:474:VAL:CG2	2.60	0.49
1:G:493:VAL:CG2	1:H:464:LEU:HD11	2.43	0.49
1:F:139:ASP:CB	1:G:75:PRO:HG2	2.38	0.49
1:A:474:VAL:O	1:A:474:VAL:CG2	2.60	0.49
1:B:144:LEU:HB3	1:B:145:PRO:HD2	1.94	0.49
1:C:23:TRP:CZ2	1:C:206:GLU:HB3	2.48	0.49
1:E:107:LEU:HD21	1:E:338:VAL:HG12	1.94	0.49
1:A:23:TRP:CZ2	1:A:206:GLU:HB3	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LEU:CD2	1:B:142:LEU:HD21	2.43	0.49
1:F:23:TRP:CZ2	1:F:206:GLU:HB3	2.48	0.49
1:G:23:TRP:CZ2	1:G:206:GLU:HB3	2.48	0.49
1:D:131:THR:HG22	1:D:132:LYS:HZ2	1.77	0.48
1:D:474:VAL:O	1:D:474:VAL:CG2	2.59	0.48
1:E:397:LEU:HD11	1:E:407:VAL:HG21	1.94	0.48
1:E:487:THR:CG2	1:E:488:THR:N	2.76	0.48
1:E:45:GLU:O	1:E:46:VAL:CG2	2.60	0.48
1:E:122:TRP:HZ3	1:E:478:HIS:CG	2.31	0.48
1:H:23:TRP:CZ2	1:H:206:GLU:HB3	2.48	0.48
1:C:144:LEU:HD13	1:C:148:VAL:HG11	1.91	0.48
1:C:437:LEU:HD11	1:C:441:LEU:HD11	1.96	0.48
1:D:107:LEU:HD21	1:D:338:VAL:HG12	1.94	0.48
1:E:22:GLN:O	1:E:24:VAL:HG23	2.12	0.48
1:F:394:ILE:O	1:F:394:ILE:CG2	2.59	0.48
1:H:271:LYS:HE2	1:H:397:LEU:C	2.38	0.48
1:C:146:PRO:C	1:C:148:VAL:N	2.67	0.48
1:E:23:TRP:CZ2	1:E:206:GLU:HB3	2.48	0.48
1:E:474:VAL:O	1:E:474:VAL:CG2	2.60	0.48
1:H:107:LEU:HD21	1:H:338:VAL:HG12	1.94	0.48
1:B:35:TYR:N	1:B:35:TYR:CD2	2.81	0.48
1:F:44:THR:HG1	1:F:45:GLU:H	1.62	0.48
1:H:271:LYS:CE	1:H:397:LEU:O	2.59	0.48
1:H:271:LYS:HG3	1:H:271:LYS:O	2.12	0.48
1:H:483:ILE:O	1:H:487:THR:OG1	2.31	0.48
1:A:146:PRO:C	1:A:148:VAL:N	2.69	0.48
1:A:296:ASN:O	1:A:299:GLN:HB2	2.14	0.48
1:C:144:LEU:HB3	1:C:145:PRO:CD	2.43	0.48
1:H:396:LEU:HD11	1:H:405:VAL:HG12	1.96	0.48
1:A:293:ILE:O	1:A:293:ILE:CG1	2.56	0.48
1:C:16:GLN:OE1	1:C:23:TRP:HB3	2.13	0.48
1:G:293:ILE:O	1:G:293:ILE:CG1	2.56	0.48
1:H:65:LEU:HD11	1:H:160:GLY:CA	2.41	0.48
1:D:293:ILE:O	1:D:293:ILE:CG1	2.56	0.48
1:D:296:ASN:HD22	1:D:300:VAL:HG22	1.79	0.48
1:H:474:VAL:O	1:H:474:VAL:CG2	2.59	0.47
1:F:396:LEU:HD13	1:F:407:VAL:HB	1.96	0.47
1:G:144:LEU:HB2	1:G:148:VAL:HG23	1.95	0.47
1:F:426:TYR:HB3	1:F:472:SER:OG	2.13	0.47
1:H:80:ARG:HH11	1:H:80:ARG:CG	2.25	0.47
1:H:89:LEU:HA	1:H:89:LEU:HD12	1.58	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LEU:HG	1:B:461:ASP:CB	2.44	0.47
1:E:122:TRP:CZ3	1:E:478:HIS:CG	3.02	0.47
1:H:296:ASN:O	1:H:299:GLN:HB2	2.13	0.47
1:A:487:THR:CG2	1:A:488:THR:N	2.76	0.47
1:C:322:ALA:O	1:C:326:GLU:HB2	2.15	0.47
1:E:142:LEU:CB	1:E:143:PRO:HA	2.39	0.47
1:F:35:TYR:CD2	1:F:35:TYR:N	2.81	0.47
1:G:487:THR:CG2	1:G:488:THR:N	2.76	0.47
1:A:83:LEU:CD1	1:A:127:ALA:HB1	2.44	0.47
1:A:322:ALA:O	1:A:326:GLU:HB2	2.15	0.47
1:A:459:MET:CE	1:B:144:LEU:HD21	2.38	0.47
1:B:487:THR:CG2	1:B:488:THR:N	2.76	0.47
1:E:83:LEU:CD1	1:E:127:ALA:HB1	2.44	0.47
1:G:39:THR:O	1:G:41:ASP:N	2.47	0.47
1:G:258:GLY:O	1:H:254:GLY:HA3	2.14	0.47
1:H:322:ALA:O	1:H:326:GLU:HB2	2.15	0.47
1:B:322:ALA:O	1:B:326:GLU:HB2	2.15	0.47
1:G:109:ILE:HG13	1:G:110:TYR:H	1.80	0.47
1:G:392:LYS:O	1:G:394:ILE:N	2.48	0.47
1:H:271:LYS:HE2	1:H:397:LEU:HA	1.97	0.47
1:B:166:ILE:O	1:B:166:ILE:HG13	2.15	0.47
1:D:185:CYS:HB2	1:D:187:ASN:ND2	2.30	0.47
1:E:185:CYS:HB2	1:E:187:ASN:ND2	2.30	0.47
1:A:459:MET:HE3	1:B:144:LEU:CD2	2.38	0.47
1:B:185:CYS:HB2	1:B:187:ASN:ND2	2.30	0.47
1:B:371:THR:O	1:B:371:THR:CG2	2.43	0.47
1:A:372:GLU:O	1:A:374:PRO:HD3	2.15	0.46
1:C:46:VAL:CG1	1:C:47:PRO:CD	2.94	0.46
1:C:276:VAL:HB	1:C:309:VAL:HG13	1.97	0.46
1:G:166:ILE:O	1:G:166:ILE:HG13	2.15	0.46
1:H:293:ILE:O	1:H:293:ILE:CG1	2.56	0.46
1:C:258:GLY:O	1:D:254:GLY:HA3	2.14	0.46
1:D:64:THR:C	1:D:67:SER:HB2	2.40	0.46
1:D:274:VAL:HG22	1:D:307:LEU:HD12	1.98	0.46
1:A:122:TRP:CZ3	1:A:478:HIS:CG	3.02	0.46
1:D:483:ILE:O	1:D:483:ILE:CG2	2.57	0.46
1:E:276:VAL:HB	1:E:309:VAL:HG13	1.97	0.46
1:F:44:THR:OG1	1:F:45:GLU:N	2.47	0.46
1:C:293:ILE:O	1:C:293:ILE:CG1	2.56	0.46
1:D:373:ALA:HA	1:D:374:PRO:HD3	1.80	0.46
1:E:44:THR:OG1	1:E:45:GLU:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:ILE:O	1:E:166:ILE:HG13	2.15	0.46
1:F:322:ALA:O	1:F:326:GLU:HB2	2.15	0.46
1:G:46:VAL:HG12	1:G:47:PRO:HD2	1.97	0.46
1:A:45:GLU:C	1:A:46:VAL:CG2	2.87	0.46
1:A:75:PRO:CB	1:D:139:ASP:OD2	2.64	0.46
1:A:276:VAL:HB	1:A:309:VAL:HG13	1.97	0.46
1:B:170:PHE:N	1:B:171:PRO:HD3	2.31	0.46
1:D:322:ALA:O	1:D:326:GLU:HB2	2.15	0.46
1:E:45:GLU:C	1:E:46:VAL:CG2	2.87	0.46
1:E:281:ASP:HA	1:E:282:PRO:HD2	1.78	0.46
1:E:322:ALA:O	1:E:326:GLU:HB2	2.15	0.46
1:E:390:GLU:O	1:E:391:LYS:C	2.59	0.46
1:G:144:LEU:C	1:G:145:PRO:O	2.54	0.46
1:G:362:ASP:HB3	1:G:394:ILE:HG22	1.97	0.46
1:A:148:VAL:HG12	1:A:149:ARG:N	2.30	0.46
1:A:170:PHE:N	1:A:171:PRO:HD3	2.31	0.46
1:A:392:LYS:O	1:A:394:ILE:HD13	2.15	0.46
1:B:274:VAL:HG22	1:B:307:LEU:HD12	1.98	0.46
1:F:170:PHE:N	1:F:171:PRO:HD3	2.31	0.46
1:H:185:CYS:HB2	1:H:187:ASN:ND2	2.30	0.46
1:B:46:VAL:HG12	1:B:47:PRO:HD2	1.98	0.46
1:C:109:ILE:HG13	1:C:110:TYR:H	1.80	0.46
1:F:185:CYS:HB2	1:F:187:ASN:ND2	2.30	0.46
1:G:416:GLU:O	1:G:420:GLU:HG2	2.16	0.46
1:B:170:PHE:HB2	1:B:174:MET:HG2	1.98	0.46
1:G:322:ALA:O	1:G:326:GLU:HB2	2.15	0.46
1:H:64:THR:C	1:H:67:SER:HB2	2.40	0.46
1:H:274:VAL:HG22	1:H:307:LEU:HD12	1.98	0.46
1:C:170:PHE:N	1:C:171:PRO:HD3	2.31	0.46
1:D:166:ILE:O	1:D:166:ILE:HG13	2.15	0.46
1:E:142:LEU:HD12	1:E:144:LEU:HG	1.97	0.46
1:E:170:PHE:N	1:E:171:PRO:HD3	2.31	0.46
1:G:276:VAL:HB	1:G:309:VAL:HG13	1.97	0.46
1:H:276:VAL:HB	1:H:309:VAL:HG13	1.98	0.46
1:H:443:ILE:HD13	1:H:443:ILE:HA	1.64	0.46
1:F:18:LEU:C	1:F:19:ILE:HG13	2.41	0.46
1:F:46:VAL:CG1	1:F:47:PRO:CD	2.94	0.46
1:F:276:VAL:HB	1:F:309:VAL:HG13	1.97	0.46
1:G:185:CYS:HB2	1:G:187:ASN:ND2	2.30	0.46
1:H:166:ILE:O	1:H:166:ILE:HG13	2.15	0.46
1:A:241:VAL:HG13	1:A:257:CYS:SG	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:VAL:HB	1:B:309:VAL:HG13	1.98	0.45
1:C:166:ILE:O	1:C:166:ILE:HG13	2.15	0.45
1:D:18:LEU:C	1:D:19:ILE:HG13	2.41	0.45
1:D:276:VAL:HB	1:D:309:VAL:HG13	1.98	0.45
1:E:129:TRP:C	1:E:131:THR:H	2.25	0.45
1:G:46:VAL:CG1	1:G:47:PRO:CD	2.93	0.45
1:A:129:TRP:HA	1:A:129:TRP:CE3	2.52	0.45
1:A:170:PHE:HB2	1:A:174:MET:HG2	1.98	0.45
1:C:18:LEU:C	1:C:19:ILE:HG13	2.41	0.45
1:C:487:THR:CG2	1:C:488:THR:N	2.76	0.45
1:H:170:PHE:HB2	1:H:174:MET:HG2	1.98	0.45
1:A:142:LEU:CD1	1:A:144:LEU:HG	2.47	0.45
1:B:46:VAL:CG1	1:B:47:PRO:CD	2.94	0.45
1:C:416:GLU:O	1:C:420:GLU:HG2	2.16	0.45
1:H:18:LEU:C	1:H:19:ILE:HG13	2.41	0.45
1:A:129:TRP:C	1:A:131:THR:H	2.25	0.45
1:A:241:VAL:HG21	1:A:253:ILE:HG21	1.99	0.45
1:A:274:VAL:HG22	1:A:307:LEU:HD12	1.98	0.45
1:B:34:VAL:CG1	1:B:103:ASN:HD21	2.30	0.45
1:F:34:VAL:CG1	1:F:103:ASN:HD21	2.30	0.45
1:A:75:PRO:CG	1:D:139:ASP:HB2	2.37	0.45
1:A:281:ASP:HA	1:A:282:PRO:HD2	1.78	0.45
1:A:296:ASN:ND2	1:A:299:GLN:O	2.48	0.45
1:D:34:VAL:CG1	1:D:103:ASN:HD21	2.30	0.45
1:D:358:ASN:HD22	1:D:358:ASN:C	2.24	0.45
1:G:274:VAL:HG22	1:G:307:LEU:HD12	1.98	0.45
1:H:139:ASP:OD1	1:H:139:ASP:C	2.57	0.45
1:H:170:PHE:N	1:H:171:PRO:HD3	2.31	0.45
1:H:425:VAL:CG1	1:H:471:ASP:OD2	2.65	0.45
1:A:454:VAL:HB	1:B:494:ILE:HG23	1.99	0.45
1:E:454:VAL:HB	1:F:494:ILE:HG23	1.99	0.45
1:A:427:GLY:O	1:A:449:ALA:HA	2.17	0.45
1:C:46:VAL:HG12	1:C:47:PRO:HD2	1.97	0.45
1:C:413:ASP:OD1	1:C:416:GLU:CB	2.64	0.45
1:D:170:PHE:N	1:D:171:PRO:HD3	2.31	0.45
1:F:274:VAL:HG22	1:F:307:LEU:HD12	1.98	0.45
1:G:44:THR:OG1	1:G:45:GLU:N	2.48	0.45
1:H:34:VAL:CG1	1:H:103:ASN:HD21	2.30	0.45
1:B:18:LEU:C	1:B:19:ILE:HG13	2.41	0.45
1:B:180:ALA:HB3	1:B:181:PRO:HD3	1.99	0.45
1:D:394:ILE:O	1:D:395:ARG:CB	2.65	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:437:LEU:HD21	1:G:494:ILE:HG21	1.98	0.45
1:A:122:TRP:CH2	1:A:478:HIS:CE1	3.05	0.45
1:C:274:VAL:HG22	1:C:307:LEU:HD12	1.98	0.45
1:D:189:VAL:HG22	1:D:218:LEU:HD23	1.99	0.45
1:F:373:ALA:HA	1:F:374:PRO:HD3	1.80	0.45
1:B:180:ALA:CB	1:B:181:PRO:CD	2.95	0.45
1:C:281:ASP:HA	1:C:282:PRO:HD2	1.78	0.45
1:G:360:ILE:HD13	1:G:360:ILE:HG21	1.66	0.45
1:H:80:ARG:CG	1:H:80:ARG:NH1	2.80	0.45
1:D:89:LEU:HA	1:D:89:LEU:HD12	1.57	0.44
1:E:122:TRP:CH2	1:E:478:HIS:CE1	3.05	0.44
1:G:277:LEU:HD12	1:G:434:THR:HB	1.99	0.44
1:H:180:ALA:CB	1:H:181:PRO:CD	2.95	0.44
1:A:180:ALA:HB3	1:A:181:PRO:HD3	1.99	0.44
1:E:362:ASP:OD2	1:E:394:ILE:O	2.34	0.44
1:G:108:LEU:HD22	1:G:334:LEU:CD2	2.48	0.44
1:G:143:PRO:HD2	1:G:143:PRO:O	2.17	0.44
1:C:170:PHE:HB2	1:C:174:MET:HG2	1.98	0.44
1:E:108:LEU:HD22	1:E:334:LEU:CD2	2.47	0.44
1:E:274:VAL:HG22	1:E:307:LEU:HD12	1.97	0.44
1:F:46:VAL:HG12	1:F:47:PRO:HD2	1.98	0.44
1:F:170:PHE:HB2	1:F:174:MET:HG2	1.98	0.44
1:F:180:ALA:CB	1:F:181:PRO:CD	2.95	0.44
1:G:64:THR:HA	1:G:67:SER:HB2	2.00	0.44
1:A:74:PRO:HA	1:A:75:PRO:HD3	1.88	0.44
1:B:247:THR:HB	1:B:269:GLY:H	1.83	0.44
1:B:281:ASP:HB3	1:B:284:GLU:HB2	2.00	0.44
1:C:108:LEU:HD22	1:C:334:LEU:CD2	2.48	0.44
1:D:180:ALA:HB3	1:D:181:PRO:HD3	1.99	0.44
1:F:394:ILE:HG22	1:F:396:LEU:H	1.83	0.44
1:H:189:VAL:HG22	1:H:218:LEU:HD23	1.99	0.44
1:F:277:LEU:HD12	1:F:434:THR:CB	2.48	0.44
1:G:34:VAL:CG1	1:G:103:ASN:HD21	2.30	0.44
1:A:437:LEU:CD2	1:A:441:LEU:HD12	2.48	0.44
1:C:64:THR:HA	1:C:67:SER:HB2	1.99	0.44
1:B:108:LEU:HD22	1:B:334:LEU:CD2	2.47	0.44
1:B:139:ASP:O	1:B:140:LEU:HD12	2.09	0.44
1:G:64:THR:O	1:G:67:SER:CB	2.66	0.44
1:A:122:TRP:HZ3	1:A:478:HIS:CG	2.31	0.44
1:B:496:TYR:O	1:D:442:ARG:NH2	2.47	0.44
1:C:180:ALA:HB3	1:C:181:PRO:HD3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:VAL:O	1:C:474:VAL:CG1	2.65	0.44
1:D:108:LEU:HD22	1:D:334:LEU:CD2	2.47	0.44
1:D:170:PHE:HB2	1:D:174:MET:HG2	1.98	0.44
1:E:129:TRP:HA	1:E:129:TRP:CE3	2.52	0.44
1:E:170:PHE:HB2	1:E:174:MET:HG2	1.98	0.44
1:A:166:ILE:O	1:A:166:ILE:HG13	2.15	0.44
1:D:82:LEU:HB3	1:D:127:ALA:HB2	2.00	0.44
1:D:180:ALA:HB3	1:D:181:PRO:HD2	2.00	0.44
1:D:401:VAL:O	1:D:402:PHE:CB	2.66	0.44
1:E:401:VAL:O	1:E:402:PHE:CB	2.66	0.44
1:H:17:MET:HG2	1:H:47:PRO:HG2	2.00	0.44
1:A:360:ILE:HD13	1:A:360:ILE:HG21	1.66	0.43
1:B:373:ALA:HA	1:B:374:PRO:HD3	1.80	0.43
1:C:34:VAL:CG1	1:C:103:ASN:HD21	2.30	0.43
1:E:180:ALA:HB3	1:E:181:PRO:HD2	2.00	0.43
1:E:180:ALA:CB	1:E:181:PRO:CD	2.95	0.43
1:G:144:LEU:O	1:G:145:PRO:O	2.36	0.43
1:G:180:ALA:CB	1:G:181:PRO:CD	2.95	0.43
1:H:180:ALA:HB3	1:H:181:PRO:HD2	2.00	0.43
1:H:373:ALA:HA	1:H:374:PRO:HD3	1.81	0.43
1:A:324:ILE:HD13	1:A:324:ILE:HG21	1.60	0.43
1:D:17:MET:HG2	1:D:47:PRO:HG2	2.00	0.43
1:F:180:ALA:HB3	1:F:181:PRO:HD3	1.99	0.43
1:F:494:ILE:CG2	1:H:437:LEU:HD21	2.48	0.43
1:H:247:THR:CA	1:H:268:LEU:HB3	2.48	0.43
1:A:277:LEU:HD12	1:A:434:THR:CB	2.48	0.43
1:F:293:ILE:O	1:F:293:ILE:CG1	2.56	0.43
1:G:18:LEU:C	1:G:19:ILE:HG13	2.41	0.43
1:G:251:ARG:HG2	1:H:259:ARG:O	2.18	0.43
1:H:180:ALA:HB3	1:H:181:PRO:HD3	1.99	0.43
1:H:306:ARG:HD3	1:H:397:LEU:HD12	2.00	0.43
1:A:146:PRO:O	1:A:148:VAL:HG23	2.19	0.43
1:B:243:PHE:HE2	1:B:268:LEU:CD2	2.32	0.43
1:C:277:LEU:HD12	1:C:434:THR:HB	1.98	0.43
1:E:139:ASP:O	1:E:140:LEU:HG	2.17	0.43
1:E:394:ILE:HD12	1:E:394:ILE:HA	1.83	0.43
1:G:144:LEU:O	1:G:145:PRO:C	2.56	0.43
1:G:180:ALA:HB3	1:G:181:PRO:HD2	2.00	0.43
1:G:180:ALA:HB3	1:G:181:PRO:HD3	1.99	0.43
1:H:82:LEU:HB3	1:H:127:ALA:HB2	2.00	0.43
1:H:247:THR:HG21	1:H:426:TYR:CE1	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:LEU:HB2	1:B:334:LEU:HD23	2.00	0.43
1:D:108:LEU:HB2	1:D:334:LEU:HD23	2.00	0.43
1:A:145:PRO:O	1:A:148:VAL:HB	2.19	0.43
1:A:397:LEU:HD11	1:A:407:VAL:HG21	2.01	0.43
1:B:277:LEU:HD12	1:B:434:THR:CB	2.48	0.43
1:D:180:ALA:CB	1:D:181:PRO:CD	2.95	0.43
1:E:108:LEU:HB2	1:E:334:LEU:HD23	2.00	0.43
1:E:113:LEU:N	1:E:113:LEU:CD2	2.80	0.43
1:F:437:LEU:CD2	1:F:441:LEU:HD12	2.48	0.43
1:H:401:VAL:O	1:H:402:PHE:CB	2.66	0.43
1:B:180:ALA:HB3	1:B:181:PRO:HD2	2.00	0.43
1:B:247:THR:CA	1:B:268:LEU:HB3	2.49	0.43
1:E:277:LEU:HD12	1:E:434:THR:CB	2.48	0.43
1:F:142:LEU:CB	1:F:143:PRO:CA	2.88	0.43
1:F:477:GLU:HG3	1:F:478:HIS:CE1	2.54	0.43
1:H:108:LEU:HD22	1:H:334:LEU:CD2	2.48	0.43
1:H:324:ILE:HD13	1:H:324:ILE:HG21	1.60	0.43
1:A:397:LEU:CD1	1:A:407:VAL:HG21	2.49	0.43
1:B:360:ILE:HD13	1:B:360:ILE:HG21	1.66	0.43
1:B:401:VAL:O	1:B:402:PHE:CB	2.66	0.43
1:E:139:ASP:C	1:E:140:LEU:CG	2.92	0.43
1:E:437:LEU:HD21	1:G:494:ILE:CG2	2.49	0.43
1:G:401:VAL:O	1:G:402:PHE:CB	2.66	0.43
1:E:180:ALA:HB3	1:E:181:PRO:HD3	1.99	0.43
1:G:74:PRO:HA	1:G:75:PRO:HD3	1.87	0.43
1:A:401:VAL:O	1:A:402:PHE:CB	2.66	0.42
1:E:426:TYR:CD1	1:E:471:ASP:HB3	2.54	0.42
1:F:74:PRO:HA	1:F:75:PRO:HD3	1.88	0.42
1:F:225:GLY:C	1:F:227:THR:N	2.74	0.42
1:B:477:GLU:HG3	1:B:478:HIS:CE1	2.54	0.42
1:C:108:LEU:HB2	1:C:334:LEU:HD23	2.00	0.42
1:C:251:ARG:HG2	1:D:259:ARG:O	2.18	0.42
1:C:388:ASN:O	1:C:388:ASN:CG	2.59	0.42
1:D:360:ILE:HG21	1:D:360:ILE:HD13	1.66	0.42
1:E:168:TRP:HE3	1:E:344:VAL:HG21	1.85	0.42
1:G:388:ASN:O	1:G:388:ASN:CG	2.59	0.42
1:B:247:THR:HA	1:B:268:LEU:HD22	2.02	0.42
1:C:180:ALA:HB3	1:C:181:PRO:HD2	2.00	0.42
1:G:109:ILE:HG13	1:G:110:TYR:N	2.35	0.42
1:H:168:TRP:HE3	1:H:344:VAL:HG21	1.85	0.42
1:C:433:TRP:O	1:C:434:THR:HB	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:THR:OG1	1:D:45:GLU:N	2.48	0.42
1:D:483:ILE:O	1:D:487:THR:OG1	2.31	0.42
1:E:185:CYS:HB2	1:E:187:ASN:HD22	1.85	0.42
1:F:168:TRP:HE3	1:F:344:VAL:HG21	1.85	0.42
1:B:393:ASP:C	1:B:394:ILE:O	2.56	0.42
1:B:450:GLY:C	1:B:451:THR:HG23	2.45	0.42
1:E:17:MET:CE	1:E:47:PRO:HB2	2.50	0.42
1:E:74:PRO:HA	1:E:75:PRO:HD3	1.88	0.42
1:G:46:VAL:HG11	1:G:222:THR:HG21	2.02	0.42
1:G:170:PHE:N	1:G:171:PRO:HD3	2.35	0.42
1:B:168:TRP:HE3	1:B:344:VAL:HG21	1.85	0.42
1:C:180:ALA:CB	1:C:181:PRO:CD	2.95	0.42
1:D:74:PRO:HA	1:D:75:PRO:HD3	1.88	0.42
1:E:293:ILE:O	1:E:293:ILE:CG1	2.56	0.42
1:B:437:LEU:HD21	1:D:494:ILE:HG21	2.02	0.42
1:E:17:MET:HE2	1:E:47:PRO:CB	2.50	0.42
1:E:55:ASN:OD1	1:E:55:ASN:O	2.37	0.42
1:E:139:ASP:HB2	1:H:75:PRO:CG	2.34	0.42
1:F:180:ALA:HB3	1:F:181:PRO:HD2	2.00	0.42
1:G:108:LEU:HB2	1:G:334:LEU:HD23	2.00	0.42
1:A:17:MET:CE	1:A:47:PRO:HB2	2.50	0.42
1:A:55:ASN:OD1	1:A:55:ASN:C	2.63	0.42
1:A:55:ASN:OD1	1:A:55:ASN:O	2.38	0.42
1:A:241:VAL:CG2	1:A:264:VAL:HG23	2.43	0.42
1:F:79:GLU:OE2	1:F:131:THR:HG21	2.20	0.42
1:F:166:ILE:O	1:F:166:ILE:HG13	2.15	0.42
1:A:168:TRP:HE3	1:A:344:VAL:HG21	1.85	0.41
1:B:79:GLU:OE2	1:B:131:THR:HG21	2.20	0.41
1:C:428:LEU:HD12	1:C:468:GLY:HA3	2.02	0.41
1:C:437:LEU:CD1	1:C:441:LEU:HD11	2.50	0.41
1:D:80:ARG:CG	1:D:80:ARG:NH1	2.80	0.41
1:G:185:CYS:HB2	1:G:187:ASN:HD22	1.85	0.41
1:H:360:ILE:HG21	1:H:360:ILE:HD13	1.66	0.41
1:A:123:LEU:O	1:A:124:ARG:C	2.63	0.41
1:A:180:ALA:CB	1:A:181:PRO:CD	2.95	0.41
1:C:394:ILE:O	1:C:397:LEU:HD12	2.20	0.41
1:E:123:LEU:O	1:E:124:ARG:C	2.63	0.41
1:G:394:ILE:O	1:G:397:LEU:HD12	2.20	0.41
1:H:119:SER:HB3	1:H:176:VAL:HG21	2.02	0.41
1:A:119:SER:HB3	1:A:176:VAL:HG21	2.02	0.41
1:A:180:ALA:HB3	1:A:181:PRO:HD2	2.00	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:THR:HA	1:B:67:SER:HB2	2.02	0.41
1:C:324:ILE:HG21	1:C:324:ILE:HD13	1.60	0.41
1:D:394:ILE:HG13	1:D:395:ARG:N	2.34	0.41
1:E:55:ASN:OD1	1:E:55:ASN:C	2.63	0.41
1:E:83:LEU:HD12	1:E:127:ALA:HB1	2.02	0.41
1:G:247:THR:CA	1:G:268:LEU:HB3	2.48	0.41
1:C:119:SER:HB3	1:C:176:VAL:HG21	2.02	0.41
1:C:123:LEU:O	1:C:124:ARG:C	2.63	0.41
1:F:496:TYR:CE2	1:H:441:LEU:HD23	2.55	0.41
1:G:34:VAL:HG13	1:G:103:ASN:HD21	1.86	0.41
1:A:44:THR:OG1	1:A:45:GLU:N	2.48	0.41
1:G:119:SER:HB3	1:G:176:VAL:HG21	2.02	0.41
1:G:428:LEU:HD12	1:G:468:GLY:HA3	2.01	0.41
1:H:185:CYS:HB2	1:H:187:ASN:HD22	1.85	0.41
1:A:22:GLN:C	1:A:24:VAL:HG23	2.46	0.41
1:C:44:THR:OG1	1:C:45:GLU:N	2.48	0.41
1:G:388:ASN:O	1:G:388:ASN:OD1	2.39	0.41
1:H:34:VAL:HG13	1:H:103:ASN:HD21	1.86	0.41
1:H:108:LEU:HB2	1:H:334:LEU:HD23	2.01	0.41
1:H:397:LEU:HD13	1:H:407:VAL:HG11	2.03	0.41
1:C:109:ILE:HG13	1:C:110:TYR:N	2.35	0.41
1:D:168:TRP:HE3	1:D:344:VAL:HG21	1.85	0.41
1:E:144:LEU:HD21	1:F:459:MET:HE3	2.02	0.41
1:F:75:PRO:HG2	1:G:139:ASP:HB3	2.03	0.41
1:F:397:LEU:HD13	1:F:407:VAL:HG11	2.02	0.41
1:F:401:VAL:O	1:F:402:PHE:CB	2.66	0.41
1:H:36:ASN:O	1:H:40:GLY:N	2.52	0.41
1:A:17:MET:HE2	1:A:47:PRO:CB	2.50	0.41
1:B:46:VAL:HG11	1:B:222:THR:HG21	2.02	0.41
1:B:496:TYR:CE2	1:D:441:LEU:HD23	2.55	0.41
1:C:46:VAL:HG11	1:C:222:THR:HG21	2.02	0.41
1:C:145:PRO:HB2	1:C:148:VAL:HG21	2.03	0.41
1:E:427:GLY:O	1:E:449:ALA:HA	2.21	0.41
1:G:166:ILE:CG1	1:G:193:PRO:HA	2.44	0.41
1:G:324:ILE:HG21	1:G:324:ILE:HD13	1.60	0.41
1:A:83:LEU:HD12	1:A:127:ALA:CB	2.50	0.41
1:A:416:GLU:O	1:A:420:GLU:HG2	2.20	0.41
1:C:129:TRP:CG	1:C:483:ILE:HD11	2.55	0.41
1:D:65:LEU:HD11	1:D:160:GLY:CA	2.43	0.41
1:D:277:LEU:HD12	1:D:434:THR:HB	2.02	0.41
1:F:123:LEU:O	1:F:124:ARG:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:247:THR:CA	1:F:268:LEU:HB3	2.48	0.41
1:H:277:LEU:HD12	1:H:434:THR:HB	2.02	0.41
1:B:144:LEU:HB3	1:B:145:PRO:CD	2.51	0.41
1:B:144:LEU:HD23	1:B:144:LEU:HA	1.86	0.41
1:C:34:VAL:HG13	1:C:103:ASN:HD21	1.86	0.41
1:C:46:VAL:HG12	1:C:47:PRO:CD	2.51	0.41
1:C:144:LEU:CB	1:C:148:VAL:HG12	2.50	0.41
1:D:119:SER:HB3	1:D:176:VAL:HG21	2.02	0.41
1:E:324:ILE:HD13	1:E:324:ILE:HG21	1.60	0.41
1:G:46:VAL:HG12	1:G:47:PRO:CD	2.51	0.41
1:G:143:PRO:O	1:G:143:PRO:CD	2.69	0.41
1:H:306:ARG:CD	1:H:397:LEU:HD12	2.51	0.41
1:A:142:LEU:HD13	1:A:144:LEU:CG	2.49	0.40
1:B:119:SER:OG	1:B:173:LEU:HD12	2.21	0.40
1:C:247:THR:CA	1:C:268:LEU:HB3	2.48	0.40
1:C:443:ILE:HD13	1:C:443:ILE:HG21	1.72	0.40
1:D:185:CYS:HB2	1:D:187:ASN:HD22	1.85	0.40
1:D:426:TYR:CD1	1:D:471:ASP:HB3	2.56	0.40
1:E:83:LEU:HD12	1:E:127:ALA:CB	2.50	0.40
1:A:18:LEU:HD22	1:A:205:ALA:HB1	2.03	0.40
1:B:34:VAL:HG13	1:B:103:ASN:HD21	1.86	0.40
1:B:179:ILE:HG22	1:B:189:VAL:HG21	2.03	0.40
1:B:296:ASN:O	1:B:299:GLN:HB2	2.21	0.40
1:B:320:ARG:HD3	1:B:320:ARG:HH11	1.77	0.40
1:C:388:ASN:O	1:C:388:ASN:OD1	2.39	0.40
1:C:401:VAL:O	1:C:402:PHE:CB	2.66	0.40
1:F:34:VAL:HG13	1:F:103:ASN:HD21	1.86	0.40
1:F:45:GLU:C	1:F:46:VAL:HG23	2.47	0.40
1:F:64:THR:HA	1:F:67:SER:HB2	2.02	0.40
1:G:281:ASP:HA	1:G:282:PRO:HD2	1.78	0.40
1:A:45:GLU:O	1:A:46:VAL:HG22	2.22	0.40
1:A:247:THR:CA	1:A:268:LEU:HB3	2.48	0.40
1:B:46:VAL:HG12	1:B:47:PRO:CD	2.52	0.40
1:C:45:GLU:C	1:C:46:VAL:HG23	2.47	0.40
1:C:185:CYS:HB2	1:C:187:ASN:ND2	2.35	0.40
1:F:46:VAL:HG11	1:F:222:THR:HG21	2.02	0.40
1:A:51:VAL:O	1:A:51:VAL:CG1	2.70	0.40
1:A:83:LEU:HD12	1:A:127:ALA:HB1	2.02	0.40
1:E:22:GLN:C	1:E:24:VAL:HG23	2.45	0.40
1:E:258:GLY:O	1:F:254:GLY:HA3	2.22	0.40
1:E:494:ILE:HG23	1:F:454:VAL:HB	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:VAL:O	1:G:51:VAL:CG1	2.70	0.40
1:G:168:TRP:HE3	1:G:344:VAL:HG21	1.85	0.40
1:C:146:PRO:O	1:C:148:VAL:N	2.55	0.40
1:C:373:ALA:HA	1:C:374:PRO:HD3	1.80	0.40
1:E:119:SER:HB3	1:E:176:VAL:HG21	2.02	0.40
1:G:129:TRP:CE3	1:G:129:TRP:HA	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	479/516 (93%)	440 (92%)	36 (8%)	3 (1%)	21	39
1	B	479/516 (93%)	429 (90%)	46 (10%)	4 (1%)	16	31
1	C	479/516 (93%)	439 (92%)	36 (8%)	4 (1%)	16	31
1	D	479/516 (93%)	434 (91%)	42 (9%)	3 (1%)	21	39
1	E	479/516 (93%)	439 (92%)	38 (8%)	2 (0%)	30	48
1	F	479/516 (93%)	433 (90%)	43 (9%)	3 (1%)	21	39
1	G	479/516 (93%)	439 (92%)	38 (8%)	2 (0%)	30	48
1	H	479/516 (93%)	436 (91%)	39 (8%)	4 (1%)	16	31
All	All	3832/4128 (93%)	3489 (91%)	318 (8%)	25 (1%)	18	35

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	PRO
1	C	143	PRO
1	D	143	PRO
1	F	143	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	394	ILE
1	B	297	HIS
1	C	142	LEU
1	E	144	LEU
1	B	142	LEU
1	H	142	LEU
1	C	145	PRO
1	D	142	LEU
1	A	198	PRO
1	B	198	PRO
1	C	198	PRO
1	D	198	PRO
1	E	198	PRO
1	F	142	LEU
1	F	198	PRO
1	G	198	PRO
1	H	198	PRO
1	H	394	ILE
1	B	143	PRO
1	H	143	PRO
1	G	143	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	338/408 (83%)	311 (92%)	27 (8%)	11	24
1	B	337/408 (83%)	311 (92%)	26 (8%)	12	26
1	C	336/408 (82%)	310 (92%)	26 (8%)	12	26
1	D	338/408 (83%)	277 (82%)	61 (18%)	2	3
1	E	336/408 (82%)	313 (93%)	23 (7%)	14	31
1	F	337/408 (83%)	311 (92%)	26 (8%)	12	26
1	G	338/408 (83%)	308 (91%)	30 (9%)	9	20
1	H	337/408 (83%)	281 (83%)	56 (17%)	2	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2697/3264 (83%)	2422 (90%)	275 (10%)	7 15

All (275) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	GLU
1	A	89	LEU
1	A	91	VAL
1	A	106	LYS
1	A	129	TRP
1	A	138	LEU
1	A	140	LEU
1	A	141	SER
1	A	166	ILE
1	A	189	VAL
1	A	196	GLU
1	A	200	THR
1	A	206	GLU
1	A	241	VAL
1	A	268	LEU
1	A	274	VAL
1	A	297	HIS
1	A	313	ILE
1	A	327	SER
1	A	334	LEU
1	A	340	MET
1	A	361	GLU
1	A	368	CYS
1	A	394	ILE
1	A	397	LEU
1	A	414	ILE
1	A	418	VAL
1	B	47	PRO
1	B	55	ASN
1	B	89	LEU
1	B	91	VAL
1	B	106	LYS
1	B	122	TRP
1	B	138	LEU
1	B	140	LEU
1	B	166	ILE
1	B	189	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	196	GLU
1	B	200	THR
1	B	206	GLU
1	B	222	THR
1	B	251	ARG
1	B	271	LYS
1	B	274	VAL
1	B	297	HIS
1	B	313	ILE
1	B	327	SER
1	B	340	MET
1	B	371	THR
1	B	396	LEU
1	B	397	LEU
1	B	414	ILE
1	B	418	VAL
1	C	47	PRO
1	C	55	ASN
1	C	65	LEU
1	C	91	VAL
1	C	106	LYS
1	C	122	TRP
1	C	129	TRP
1	C	138	LEU
1	C	140	LEU
1	C	166	ILE
1	C	189	VAL
1	C	196	GLU
1	C	200	THR
1	C	206	GLU
1	C	222	THR
1	C	268	LEU
1	C	274	VAL
1	C	297	HIS
1	C	313	ILE
1	C	327	SER
1	C	340	MET
1	C	414	ILE
1	C	416	GLU
1	C	418	VAL
1	C	419	ASN
1	C	477	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	16	GLN
1	D	22	GLN
1	D	24	VAL
1	D	32	LEU
1	D	39	THR
1	D	43	LEU
1	D	46	VAL
1	D	47	PRO
1	D	55	ASN
1	D	65	LEU
1	D	67	SER
1	D	80	ARG
1	D	82	LEU
1	D	83	LEU
1	D	84	ARG
1	D	89	LEU
1	D	91	VAL
1	D	106	LYS
1	D	122	TRP
1	D	129	TRP
1	D	131	THR
1	D	137	THR
1	D	138	LEU
1	D	141	SER
1	D	148	VAL
1	D	166	ILE
1	D	189	VAL
1	D	196	GLU
1	D	200	THR
1	D	206	GLU
1	D	218	LEU
1	D	222	THR
1	D	247	THR
1	D	251	ARG
1	D	265	SER
1	D	268	LEU
1	D	271	LYS
1	D	274	VAL
1	D	297	HIS
1	D	305	SER
1	D	313	ILE
1	D	321	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	327	SER
1	D	340	MET
1	D	365	ASP
1	D	367	ILE
1	D	371	THR
1	D	389	ARG
1	D	397	LEU
1	D	400	GLU
1	D	413	ASP
1	D	414	ILE
1	D	416	GLU
1	D	418	VAL
1	D	425	VAL
1	D	426	TYR
1	D	437	LEU
1	D	438	SER
1	D	441	LEU
1	D	464	LEU
1	D	477	GLU
1	E	79	GLU
1	E	89	LEU
1	E	91	VAL
1	E	106	LYS
1	E	113	LEU
1	E	129	TRP
1	E	141	SER
1	E	166	ILE
1	E	189	VAL
1	E	196	GLU
1	E	200	THR
1	E	206	GLU
1	E	268	LEU
1	E	274	VAL
1	E	297	HIS
1	E	313	ILE
1	E	327	SER
1	E	340	MET
1	E	394	ILE
1	E	396	LEU
1	E	397	LEU
1	E	414	ILE
1	E	418	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	17	MET
1	F	47	PRO
1	F	55	ASN
1	F	89	LEU
1	F	91	VAL
1	F	106	LYS
1	F	122	TRP
1	F	138	LEU
1	F	166	ILE
1	F	189	VAL
1	F	196	GLU
1	F	200	THR
1	F	206	GLU
1	F	222	THR
1	F	251	ARG
1	F	268	LEU
1	F	271	LYS
1	F	274	VAL
1	F	297	HIS
1	F	313	ILE
1	F	327	SER
1	F	340	MET
1	F	396	LEU
1	F	397	LEU
1	F	414	ILE
1	F	418	VAL
1	G	47	PRO
1	G	55	ASN
1	G	91	VAL
1	G	106	LYS
1	G	122	TRP
1	G	129	TRP
1	G	138	LEU
1	G	140	LEU
1	G	141	SER
1	G	142	LEU
1	G	144	LEU
1	G	166	ILE
1	G	189	VAL
1	G	196	GLU
1	G	200	THR
1	G	206	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	222	THR
1	G	268	LEU
1	G	274	VAL
1	G	297	HIS
1	G	313	ILE
1	G	327	SER
1	G	340	MET
1	G	360	ILE
1	G	396	LEU
1	G	397	LEU
1	G	416	GLU
1	G	418	VAL
1	G	419	ASN
1	G	477	GLU
1	H	22	GLN
1	H	24	VAL
1	H	32	LEU
1	H	43	LEU
1	H	46	VAL
1	H	47	PRO
1	H	55	ASN
1	H	65	LEU
1	H	67	SER
1	H	69	THR
1	H	80	ARG
1	H	82	LEU
1	H	83	LEU
1	H	84	ARG
1	H	89	LEU
1	H	91	VAL
1	H	106	LYS
1	H	122	TRP
1	H	129	TRP
1	H	131	THR
1	H	137	THR
1	H	138	LEU
1	H	141	SER
1	H	166	ILE
1	H	189	VAL
1	H	196	GLU
1	H	200	THR
1	H	206	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	218	LEU
1	H	222	THR
1	H	227	THR
1	H	247	THR
1	H	251	ARG
1	H	265	SER
1	H	268	LEU
1	H	274	VAL
1	H	297	HIS
1	H	305	SER
1	H	313	ILE
1	H	321	LEU
1	H	327	SER
1	H	340	MET
1	H	365	ASP
1	H	367	ILE
1	H	371	THR
1	H	389	ARG
1	H	397	LEU
1	H	400	GLU
1	H	413	ASP
1	H	414	ILE
1	H	416	GLU
1	H	418	VAL
1	H	438	SER
1	H	441	LEU
1	H	464	LEU
1	H	477	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	299	GLN
1	A	319	GLN
1	A	355	HIS
1	B	103	ASN
1	B	121	GLN
1	B	299	GLN
1	B	319	GLN
1	B	355	HIS
1	C	103	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	299	GLN
1	C	319	GLN
1	C	355	HIS
1	C	478	HIS
1	D	22	GLN
1	D	103	ASN
1	D	121	GLN
1	D	296	ASN
1	D	299	GLN
1	D	319	GLN
1	D	355	HIS
1	E	121	GLN
1	E	299	GLN
1	E	319	GLN
1	E	355	HIS
1	F	103	ASN
1	F	121	GLN
1	F	299	GLN
1	F	319	GLN
1	F	478	HIS
1	G	103	ASN
1	G	296	ASN
1	G	299	GLN
1	G	319	GLN
1	G	355	HIS
1	G	478	HIS
1	H	103	ASN
1	H	299	GLN
1	H	319	GLN
1	H	355	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	481/516 (93%)	-1.36	0 100 100	16, 27, 35, 41	0
1	B	481/516 (93%)	-1.40	0 100 100	16, 25, 33, 45	0
1	C	481/516 (93%)	-1.33	0 100 100	17, 27, 37, 44	0
1	D	481/516 (93%)	-1.35	0 100 100	16, 28, 38, 44	0
1	E	481/516 (93%)	-1.38	0 100 100	17, 26, 34, 43	0
1	F	481/516 (93%)	-1.41	0 100 100	16, 25, 33, 43	0
1	G	481/516 (93%)	-1.35	0 100 100	18, 28, 35, 46	0
1	H	481/516 (93%)	-1.32	0 100 100	18, 29, 37, 45	0
All	All	3848/4128 (93%)	-1.36	0 100 100	16, 27, 36, 46	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.